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1. PURPOSE

The Monitored Geologic Repository (MGR) Waste Package Department of the Civilian Radioactive Waste Management System Management & Operating Contractor (CRWMS M&O) performed calculations to provide input for disposal of spent nuclear fuel (SNF) from the N Reactor, a graphite moderated reactor at the Department of Energy's (DOE) Hanford Site (Ref. 1). The N Reactor core was fueled with slightly enriched (0.947 wt% and 0.947 to 1.25 wt% ^{235}U in Mark IV and Mark IA fuels, respectively) U-metal clad in Zircaloy-2 (Ref. 1, Sec. 3). Both types of N Reactor SNF have been considered for disposal at the proposed Yucca Mountain site. For some WPs, the outer shell and inner shell may breach (Ref. 3) allowing the influx of water. Water in the WP will moderate neutrons, increasing the likelihood of a criticality event within the WP; and the water may, in time, gradually leach the fissile components from the WP, further affecting the neutronics of the system.

This study presents calculations of the long-term geochemical behavior of WPs containing two multi-canister overpacks (MCO) with either six baskets of Mark IA or five baskets of Mark IV intact N Reactor SNF rods (Ref. 1, Sec. 4) and two high-level waste (HLW) glass pour canisters (GPCs) arranged according to the codisposal concept (Ref. 4). The specific study objectives were to determine:

1. The extent to which fissile uranium will remain in the WP after corrosion/dissolution of the initial WP configuration

2. The extent to which fissile uranium will be carried out of the degraded WP by infiltrating water (such that internal criticality is no longer possible, but the possibility of external criticality may be enhanced)

3. The nominal chemical composition for the criticality evaluations of the WP design, and to suggest the range of parametric variations for additional evaluations.

The scope of this calculation, the chemical compositions (and subsequent criticality evaluations) of the simulations, is limited to time periods up to 6.35×10^5 years. This longer time frame is closer to the one million year time horizon recently recommended by the National Academy of Sciences to the Environmental Protection Agency for performance assessment related to a nuclear repository (Ref. 5). However, it is important to note that after 100,000 years, most of the materials of interest (fissile materials) will have either been removed from the WP, reached a steady state, or been transmuted.

This document has been prepared according to Administrative Procedure AP-3.12Q (Ref. 37), *Calculations*, and is subject to the Quality Assurance Requirements and Description (QARD) Document (Ref. 41) requirements. This calculation has been prepared in accordance with the *Technical Work Plan for: Department of Energy Spent Nuclear Fuel Work Packages* (Ref. 8).

2. METHOD

The method used for this analysis involves the following steps:

- Use of basic EQ3/6 (software package, described in Section 4.1 and in Ref. 22) capability for tracing the progress of reactions with evolution of the chemistry, which includes the estimation of the concentrations remaining in solution and the composition of the precipitated solids. (EQ3 is used to determine a starting fluid composition for EQ6 calculations; it does not simulate reaction progress.)

- Evaluation of available data on the range of dissolution rates for the materials involved, to be used as material/species input for each time step.

- Use of "solid-centered flow-through" mode (SCFT) in EQ6; in this mode, an increment of aqueous "feed" solution is added continuously to the WP system, and a like volume of the existing solution is removed, simulating a continuously-stirred tank reactor. This mode is discussed in Section 4.

- Determination of fissile material concentrations in solution as a function of time (from the output of EQ6 simulated reaction times up to 6.35×10^5 years).

- Calculation of the amount of fissile material released from the WP as a function of time (fissile material loss reduces the chance of criticality within the WP).

- Composition and amounts of solids (precipitated minerals or corrosion products, and unreacted WP materials).

This calculation used version 7.2bLV (Ref. 12) of EQ6 (Refs. 22, 23, 24, and 25). The User's Manual for 7.2bLV (Ref. 13) provides a detailed description of the code. The code retains the solid-centered flow-through (SCFT) mode developed in the previous Addendum to EQ6 (Ref. 18) and is complete, mathematically correct and technically adequate for the application. Further detail on the specific methods employed for each step is available in Section 5 of this calculation.

With regard to the development of this calculation, the control of the electronic management of data was evaluated in accordance with AP-SV.1Q, *Control of the Electronic Management of Information* (Ref. 15). The evaluation (Ref. 8) determined that current work processes and procedures are adequate for the control of electronic management of data for this activity.

3. ASSUMPTIONS

All assumptions are for preliminary design. All assumptions are used throughout Section 5.

3.1 The Enhanced Design Alternative (EDA) II waste package (Ref. 26) is assumed for disposal of N Reactor SNF. The rationale for this assumption is that the EDA II design superseded the Viability Assessment (VA) design before the N Reactor calculations began.

3.2 It is assumed that the solutions that drip into the WP will have the major ion composition of J-13 well water as given in Ref. 54 (Document Tracking Number (DTN): MO0006J13WTRCM.000), and that minor components in the solution can be approximated by Reference 6 for 6.35×10^5 years. The rationale for this assumption is that the groundwater composition is controlled largely by transport through the host rock, over pathways of hundreds of meters, and the host rock composition is not expected to change substantially over 10^6 years. The assumption that the water entering the WP can be approximated by the J-13 well water implicitly assumes that any effects of contact with the engineered materials in the drift will be minimal after a few thousand years. For a few thousand years after waste emplacement, the composition may differ because of perturbations resulting from reactions with engineered materials and from the thermal pulse. These are not taken into account in this calculation because the outer shell and inner liner are not expected to breach until after that perturbed period. Therefore, the early perturbation is not relevant to the calculations reported in this document.

3.3 It is assumed that the density of J-13 well water is 1.0 g/cm^3. The rationale of this assumption is that in dilute solutions, the density is extremely close to that for pure water and that any differences are insignificant with respect to other uncertainties in the data and calculations. Moreover, this number is used only initially in EQ3/6 to convert concentrations of dissolved substances from parts per million to molality.

3.4 It is assumed that an aqueous solution fills all voids within the waste package. The rationale for this assumption is that it provides the maximum degradation rates of WP components with the potential for precipitation of radionuclides within the WP or the flushing of radionuclides from the WP, and is therefore conservative. This assumption is justified by recent evaluations of codisposal WPs (Ref. 2) which show that degradation of the WP materials (specifically, HLW glass and steel) overwhelms the native chemistry of the incoming water (Figures 5-2 through 5-20 of Ref. 2 show pH variations of 3 to 10 in WP)

3.5 It is assumed that water will circulate freely enough in the partially degraded WP that all degraded solid products will react with each other through the aqueous solution medium. The rationale for this assumption is that it provides the most rapid aqueous degradation and is, therefore, conservative with respect to criticality.

3.6 It is assumed that data in the 25°C thermodynamic database can be used for the calculation. The rationale for this assumption is that though the initial breach of the WP may occur when the WP contents are at temperatures ≥ 50°C (Ref. 7, Figures 3-20 through 3-22), at times > 25,000 years, the WP temperatures are likely to be close to 25°C. It is further assumed that the thermodynamic database used for these calculations (data0.ymp.ROA) does not differ from the database recently qualified for project use (data0.ymp.R0) in any way that would cause a significant impact to the calculations reported in this report. The rationale for this is that the changes made in the qualification process included removal of data extrapolated to elevated temperatures, which are not of concern to this study, and the correction of numerical errors due to transcription of data from the source references. Future revisions to this document will use the qualified database, and the impact of changes can be assessed at that time.

3.7 In general it is assumed that chromium and molybdenum will oxidize fully to chromate (or dichromate) and molybdate, respectively. This assumption is based on the available thermodynamic data, which indicate that in the presence of air, the chromium and molybdenum would both oxidize to the VI valence state. Laboratory observation of the corrosion of Cr and Mo containing steels and alloys, however, indicates that any such oxidation would be extremely slow. In fact, oxidation to the VI state may not occur at a significant rate with respect to the time frame of interest, or there may exist stable Cr(III) solids that substantially lower aqueous Cr concentration. For the present analyses, the assumption is made that, over the times of concern, oxidation will occur. The rationale for this assumption is that by allowing the Cr and Mo to oxidize, the pH of the system will be lowered allowing for the removal of neutron absorbers. This is conservative for internal criticality since most of the Pu and U would remain in the waste package.

3.8 The composition of the aqueous solution that will enter the waste package will not be altered by contact with the material. The rationale for this assumption is that the water is expected to move rapidly enough through openings in the waste package materials that its residence time in the corroded barrier will be too small for significant reaction to occur. Furthermore, the water flowing through the barriers will be in contact with the corrosion products left from the barrier corrosion that created the holes initially. These corrosion products will closely resemble iron oxides and hydroxides in the overlying rock. Consequently, the water should already be close to equilibrium with these compounds and would be unaffected by further contact with them, even if flow slowed enough to permit significant reaction.

3.9 It is assumed that gases in the WP solution remain in equilibrium with the ambient atmosphere outside the WP. In other words, contact of WP fluids with the gas phase in the repository is envisioned to be sufficient to maintain equilibrium with the CO_2 and O_2 present, whether or not this is the normal atmosphere in open air or rock gas that seeps out of the adjacent tuff. Moreover, the specific partial pressures of CO_2 and O_2 of the ambient repository atmosphere are set to, respectively, $10^{-3.0}$ and $10^{-0.7}$ atm. The rationale

for the oxygen partial pressure is that it is equivalent to that in the atmosphere (Ref. 10, p. F-210). The rationale for choosing the carbon dioxide pressure is to reflect the observation that J-13 well water appears to be in equilibrium with above-atmospheric carbon dioxide levels (Ref. 9, Table 7;).

3.10 It is assumed that precipitated solids are deposited, remain in place, and are not mechanically eroded or entrained as colloids in the advected water. The rationale for this assumption is that since dissolved fissile material (U, Pu, Np) may be adsorbed on colloids (clays, iron oxides) or may be precipitated as colloids during WP degradation (Ref. 7, Sec. 3.5 and 3.6) it is conservative for internal criticality to assume that all precipitated solids, including mobile colloids, will be deposited inside the WP rather than transported out of the WP.

3.11 It is assumed that corrosion rates will not be significantly enhanced by microbiologically influenced corrosion (MIC). The bases for this assumption are that: (1) MIC will probably not occur until the repository has cooled to temperatures below 100°C (212°F) and relative humidity is above 60%, (2) although MIC may increase corrosion pit and crevice density, its effect on corrosion rate will be low, and (3) Alloy 22 has not been associated with documented cases of MIC (Ref. 7, p 3-84).

3.12 It is assumed that sufficient decay heat is retained within the WP over times of interest to cause convective circulation and mixing of the water inside the WP. The analysis that serves as the rationale for this assumption is discussed in Reference 11 (Attachment VI).

3.13 It is assumed that the reported alkalinity in analyses of J-13 well water corresponds to bicarbonate (HCO_3^-) alkalinity. Contributors to alkalinity in J-13 well water, in addition to bicarbonate, potentially include borate, phosphate, and silicate. However, at pH less than 9, the contribution of silicate will be small, and in any case the concentrations of all three of these components in J-13 well water are small. Fluoride or nitrate do not contribute to alkalinity unless a sufficiently low pH is reached. The rationale for this assumption is the observation that the calculated electrical neutrality, using the assumption, is zero, within the analytical uncertainty, as it should be. The same assumption is implicitly made in Ref. 54 (DTN: MO0006J13WTRCM.000).

3.14 It is assumed that the rate of entry of water into, as well as the rate of egress from, a WP is equal to the rate at which water drips onto the WP. The rationale for this assumption is that for most of the time frame of interest, i.e., long after the corrosion barriers become largely degraded, it is more reasonable to assume that all or most of the water will enter the degraded WP than to assume that a significant portion will instead be diverted around the remains. Diversion of the water with a consequent lower entry rate has not been represented by the present calculations.

3.15 It is assumed that the most insoluble solids for a fissile radionuclide will form. This approach is conservative with respect to internal criticality since it will lead to the

maximum retention of fissile material within the WP during EQ6 runs.

3.16 Even though up to two scrap baskets containing broken or damaged N Reactor SNF rods may be loaded inside an MCO (Ref. 1, Sec 4.41), it is assumed that each MCO contained either six baskets of Mark IA or five baskets of Mark IV intact N Reactor SNF rods (Ref.1, Table 4-1). The rationale for this assumption is that these two cases represent the highest U loading of the two MCOs in a WP and is therefore, conservative.

3.17 A number of minor assumptions have been made about the geometry of the N Reactor codisposal WP. The bases for these assumptions are outlined and referenced in the spreadsheet "N-Reactor.xls" and files "dataMIA.in" and "dataMIV.in" (Attachment III) and are also discussed in Section 5.1. These assumptions were used to represent the WP geometry with the greatest accuracy possible. Where inadequate information about WP geometry was available, or it was necessary to choose among competing representations of WP geometry, the choice that appeared to lead to the greatest precision was always chosen.

3.18 For any WP components that were described as "316" stainless steel, without indication of the carbon grade, the alloy was assumed to be the low-carbon equivalent (see Section 5.1.1 for nomenclature). The rationale for this assumption is that, in general, the carbon in the steel is totally insignificant compared to the carbon supplied by the fixed CO_2 fugacity of the EQ3/6 calculation, and to the constant influx of carbonate via J-13 well water.

3.19 The Zircaloy-2 cladding on the N Reactor fuel rods is assumed to be inert. The rationale for this assumption is that this material has low chemical reactivity at low temperatures.

3.20 For most of the calculations, fresh (unirradiated) fuel is used. This approach is used since unirradiated fuel has a higher fissile content than spent fuel which also has significant neutron absorption cross sections. Therefore, using the fresh fuel is more conservative for criticality.

3.21 Zircaloy and Zr corrosion kinetics studies (Ref. 14) revealed these materials to be resistant against chemical and biological corrosion. Recent studies on corrosion of Zircaloy-clad SNF indicate growth of oxide films for a time span of a million years to be about 7.6E-03 millimeter (0.3 mil). Given the extremely slow corrosion rate, breach of the relatively thick 20-40 mil N Reactor SNF cladding (Ref. 1, Table 3-2) during the time period of interest would probably occur only as a result of mechanical damage or defect. However, the underwater storage of N Reactor SNF has resulted in the degradation or damage of over half of the fuel assemblies (Ref. 1, Appendix C, Sec. 3). Therefore, to account for cladding defects and mechanical damage, two alternative assumptions were made regarding the fraction of the SNF that is exposed to water in the WP. In one case, it was assumed that 10% of the SNF surface area is exposed to water immediately after the WP is breached and that the cladding protects the remaining SNF from exposure to water

for the duration of the run. In the rest of the cases, it was assumed that all of the SNF is immediately exposed to water upon breach of the WP. The rationale for these assumptions is that it conservatively accounts for defects and mechanical damage during storage, shipping, or packing, and that it provides a rationale for examining the sensitivity of the results to assumptions about cladding integrity.

3.22 The most recent revision of Reference 36 gives the degradation rate of N Reactor SNF as 2.0833E-09 mol/cm^2*s. For the purpose of this study, it is assumed that the original value of 2.02546 mol/cm^2*s, upon which all the calculations are based, is correct. The basis for this assumption lies in the fact that the difference is miniscule over the time frame required for waste degradation and should, therefore, not significantly change any of the information obtained in the calculations.

3.23 When "time" or "years" are discussed in the calculation, this refers to the time or years after the waste package has been breached, allowing water to enter.

3.24 For Reference 53, the data in the DTN is adequate for what will be seen in the repository and does not need further information or qualification. The basis for this is that this is the most current data, is design related information, and subject to change.

4. USE OF COMPUTER SOFTWARE AND MODELS

This section describes the computer software used to carry out the analysis.

EQ3/6 Software Package–The EQ3/6 software package originated in the mid-1970s at Northwestern University (Ref. 22). Since 1978, Lawrence Livermore National Laboratory (LLNL) has been responsible for maintenance of EQ3/6. The software has most recently been maintained under the sponsorship of the Civilian Radioactive Waste Management Program of the United States Department of Energy (DOE). The major components of the EQ3/6 package include: EQ3NR, a speciation-solubility code; EQ6, a reaction path code which models water/rock interaction or fluid mixing in either a pure reaction progress mode or a time mode; EQPT, a data file preprocessor; EQLIB, a supporting software library; and several (>5) supporting thermodynamic data files. The software deals with the concepts of thermodynamic equilibrium, thermodynamic disequilibrium, and reaction kinetics. The supporting data files contain both standard state and activity coefficient-related data. Most of the data files support the use of the Davies or B-dot equations for the activity coefficients; two others support the use of Pitzer's equations. The temperature range of the thermodynamic data in the data files varies from 25°C only, for some species, to a full range of 0-300°C for others. EQPT takes a formatted data file (a "data0" file) and writes an unformatted near-equivalent called a "data1" file, which is actually the form read by EQ3NR and EQ6. EQ3NR is useful for analyzing groundwater chemistry data, calculating solubility limits, and determining whether certain reactions are in states of partial equilibrium or disequilibrium. EQ3NR is also required to initialize an EQ6 calculation.

EQ6 represents the consequences of exposing an aqueous solution to a set of reactants, which react irreversibly. It can also represent fluid mixing and the consequences of changes in temperature. This code operates both in a pure reaction progress frame and in a time frame. In a time frame calculation, the user specifies rate laws for the progress of the irreversible reactions. Otherwise, only relative rates are specified. EQ3NR and EQ6 use a hybrid Newton-Raphson technique to make thermodynamic calculations. This is supported by a set of algorithms that create and optimize starting values. EQ6 uses an ordinary differential equation integration algorithm to solve rate equations in time mode. The codes in the EQ3/6 package are written in FORTRAN 77 and have been developed to run under the UNIX operating system on computers ranging from workstations to supercomputers. Further information on the codes of the EQ3/6 package is provided in References 22, 23, 24, and 25.

Solid-Centered Flow-Through Mode–EQ6 Version 7.2b, as distributed by LLNL, does not contain an SCFT mode. To add this mode, it is necessary to change the EQ6 source code, and recompile the source. However, by using a variant of the "special reactant" type built into EQ6, it is possible to add the functionality of SCFT mode in a very simple and straightforward manner. This mode was added to EQ6 per Software Change Request (SCR) LSCR198 (Ref. 17), and the Software Qualification Report (SQR) for Media Number 30084-M04-001 (Ref. 18).

The new mode is induced using a new type of reactant. The EQ6 input file nomenclature for this new mode is jcode=5; in the Daveler format, it is indicated by the reactant type DISPLACER. The jcode=5 is immediately trapped and converted to jcode=2, and a flag is set to indicate the existence of the DISPLACER reactant. Apart from the input trapping, the distinction between the DISPLACER and SPECIAL reactants is seen only in one 9-line block of the EQ6 FORTRAN source code (in the reacts subroutine), where the total moles of elements in the rock plus water system (mte array) is adjusted by adding in the DISPLACER reactant, and subtracting out a commensurate amount of the total aqueous elements (mteaq array).

This new EQ6 mode acts as a substitute for the allpost/nxtinput method described in References 19 and 27.

EQ3/6 7.2bLV—EQ3/6 7.2bLV (References 12, 13, and 35) is the only version of EQ6 capable of incorporating radioactive decay, and is the only version capable of passing time-varying aqueous compositions from run to run. Although EQ6 7.2bLV was the version of EQ6 used for this calculation, these two new features were not employed.

4.1 SOFTWARE

The software package, EQ3/6, Version 7.2b (Ref 64, LLNL: UCRL-MA-110662), was approved for QA work by LLNL. An installation and testing report (Ref. 20) was written and submitted to Software Configuration Management (SCM), and the proper installation was verified, before the runs described in this calculation were made. The implementation of the SCFT mode is covered by the SCR LSCR198, and the SQR for Media Number 30084-M04-001. The SCFT addendum was installed on three of the central processing units (CPUs) identified in block 16 of the SCR, and the installation and test reports were filed and returned to SCM before the calculations were run. The version 7.2bLV (Ref. 35) of EQ6 was developed under software activity plan 10075-SAP-7.2bLV-00, the validation and test report (VTR, Ref. 12) has been reviewed and approved, and a compact disc (CD) with the software was submitted to CM. All the EQ6 runs were performed on a Sandia National Laboratory system, CPU # R433480, a Dell Optiplex G1 450 MHz Pentium II. In this study, EQ3/6 was used to provide the following:

1) A general overview, of the expected, chemical reactions
2) The degradation products from corrosion of the waste forms and canisters
3) An indication of the minerals, and their amounts, likely to precipitate within the WP.

The programs have been used within the range of parameters for which they have been verified and are therefore appropriate for the application. The software was used within its range of validation. However, some runs simulated periods of high ionic strength (1 to ~10). While EQ6 is capable of handling high ionic strengths, there is no Yucca Mountain Project (YMP)-qualified thermodynamic database with corrections for high ionic strength. To address this issue, several sensitivity tests were performed using other thermodynamic databases that have corrections for high ionic strength (Ref. 58, Sec. 5.1.2). The results of calculations relating to these tests have shown that calculations at high ionic strength, using the "data0.ymp" database, overestimate the

solubility of Pu and U, which is conservative with respect to external accumulations of these elements (see assumption 3.6).

The calculation inputs include several EQ6 database files with the file extension "ymp" and other EQ6 input files specific to different WP degradation scenarios with the extension "6i". There are several types of EQ6 output files and they are not all important for the purpose of this calculation. The most relevant EQ6 input and output files for this calculation are described further in Section 5 and can be found on the compact disc (CD) in Attachment III.

The EQ3/6 package has been verified by its present custodian, LLNL. The source codes were obtained from SCM in accordance with the Management & Operating Contractor (M&O) AP-SI.1Q procedure (Ref. 48). The code was installed on the Pentium PC according to an M&O-approved Installation and Test procedure (Ref. 20).

4.2 SOFTWARE ROUTINES

Spreadsheet analyses (Attachment III) were performed with Microsoft Excel Version 97 SR-2, installed on a PC. The specific spreadsheets used for results reported in this document, are included with the attached CD (Attachment III). All formulas in the spreadsheets are identified and labeled and they are used only one time so there is only one version. The formulas used in the spreadsheets have been checked against the formulas used for the calculations in the spreadsheet and have been found to be identical.

The volume and area of some of the WP components were calculated using the software routine volarea.exe, Version 1 provided in the attached CD (Attachment III). A listing of the code and instructions for running the program is provided in the file volarea.c also provided in Attachment III. Documentation of the volarea routine is provided in Attachment I. A change history is not provided because this is the first version of the routine. The program was written in ANSI C and compiled under Microsoft C++, Version 6.0. Besides calculating volumes and areas, the program computes moles of all materials described in the input file. (Volarea recognizes only a file named "data.in." as the input file for any particular run. The produced output file "data.out" and the input file must then be renamed, after the program runs, to a more fitting description of the data in question). The input files for N Reactor SNF WPs are included in Attachment III ("dataMIA.in" and "dataMIV.in"-either of these can be run again by changing the "dataMIA" or "dataMIV" to "data"). Besides the input file, another file is necessary to run the routine: "atwts.in." The output file provides the volume, area, and mole calculation results. The results of the volume, area and mole calculations for N Reactor Mark IA and Mark IV SNF WP components can be found in the spreadsheet "N-Reactor.xls", sheets "Mols_rct", "Void_calc", and "EDA2" (Attachment III). Also included in the attached CD are the output files "dataMIA.out" and "dataMIV.out" (from "data.out") that contain the results from volarea.

Some of the calculation results were extracted into text files using the program PP (part of the EQ6 reaction path code - Ref. 50), PP is a plotting routine, but it is also possible to extract the data from a plot in PP into a text file that can be imported into another program,

such as Microsoft Excel. PP is exempt from the requirements of procedure AP-SI.1Q (Ref. 48). Section 2.1.5 of the procedure states: "Software used solely for visual display or graphical representation of data which is used in a product which is checked and approved in accordance with applicable procedures and meets stated acceptance criteria is exempt."

4.3 MODELS

None used.

5. CALCULATION

The existing database supplied with the EQ3/6 computer package is sufficiently accurate for the purposes of this calculation. The data have been carefully scrutinized by many experts over the course of several decades and carefully selected by LLNL for incorporation into the database (Refs. 22, 23, 24, and 25). These databases are periodically updated and/or new databases added, such as the data0.ymp.R0 database, DTN: MO0009THRMODYN.001, that has recently been qualified for use on the YMP. This file was developed and qualified after the calculations reported here were performed. Future revisions of this calculation will employ the most recent qualified database (see Assumption 3.6). Every run of either EQ3 or EQ6 documents automatically which database is used. The databases include references for the sources of the data. The reader is referred to this documentation, included in the electronic files labeled data0 that accompany this calculation, for details (Attachment III). Most recent calculations of WP degradation have used a composite thermodynamic database called "data0.nuc.R8", derived from the "data0.skb" and other databases provided by LLNL. A preliminary version of "data0.ymp" (Attachment III) dated June 29, 2000, was used for this calculation. The version of data0.ymp that has been qualified (DTN: MO0009THRMDYN.001) for use on the YMP is only slightly altered (molar volumes and glass as a mineral were added to the database) from the version used for the calculations reported here. Therefore no significant impact of the qualification of the new data0.ymp file is anticipated. For more information on the revision history of the database, go to "data0.ymp" in Attachment III.

The calculations begin with selection of data for compositions, amounts, surface areas, and reaction rates of the various components of N Reactor SNF WPs. These quantities are recalculated to the form required for entry into EQ6. For example, weight percentages of elements or component oxides are converted to mole fractions of elements; degradation rates in micrometers/year are converted into moles per square centimeter per second, etc. Spreadsheets (Attachment III) provide details of these calculations, and the general procedure is also described in detail in Reference 27 (Section 4). The final part of the input to EQ6 consists of the composition of J-13 well water together with a rate of influx to the WP that corresponds to suitably chosen percolation rates into a drift and drip rate into a WP (Section 5.1.1.3). The EQ6 output provides the results representing the chemical degradation of the WP, or components thereof. Sometimes the degradation of the WP is divided into stages, e.g., degradation of HLW glass before breach and exposure of the SNF assemblies and basket materials to the water. The results include the compositions and amounts of solid products and of substances in solution. Details of the results are presented below.

5.1 CALCULATION INPUTS

5.1.1 WP Materials and Performance Parameters

This section provides a brief overview of the physical and chemical characteristics of N Reactor SNF WPs, and describes how the WP is represented in the EQ6 inputs. The conversion of the WP physical description, into parameters suitable for the EQ6 input files, is performed by the

spreadsheet "N-Reactor.xls". Additional details of the description may be found in Reference 1 and the references cited therein.

Material nomenclature for the stainless steels and carbon steels used throughout this document includes: SA-240 S31603 stainless steel (hereafter referred to as 316L stainless steel); Unified Numbering System (UNS) N06625 and SA-240 S30403 stainless steel (hereafter referred to as 304L stainless steel); SA-516 and SA-36 carbon steel (hereafter referred to as A516 carbon steel).

5.1.1.1 Physical and Chemical Form of the N Reactor SNF WP

It is convenient to consider the N Reactor SNF WP as several structural components, specifically:

1) The outer shell, consisting of Alloy 22;

2) The inner shell composed of 316L stainless steel;

3) Two, perpendicular, carbon steel (A516) A-plates which intersect to form 4 vertical compartments separating the two GPCs and the two MCOs inside the WP;

4) Two MCO stands composed of A516 carbon steel;

5) Two GPCs, the 304L containers of the solidified HLW glass;

6) Two MCOs composed of 304L stainless steel;

7) Baskets, constructed of 304 L stainless steel, five containing 54 Mark IA fuel elements each, or six containing 48 Mark IA fuel elements each; and Aluminum (Al 1100) spacers which hold the fuel elements in place, all of which are inside each MCO.

8) The N Reactor (U-metal) Mark IA or Mark IV SNF rods.

The details of each of the above numbered components are in the spreadsheet "N Reactor.xls" in sheets "Glass_canisters", "EDA2", "Void_calc" and "Mols_rct" (Attachment III) and the volarea input and output files ("dataMIA.in", "dataMIV.in", "dataMIA.out" and "dataMIV.out") (Attachment III); as well as in Reference 1 (Sections 3 and 4).

Table 1 provides a summary of the compositions of the principal steel alloys used in the calculations. In Table 1 and all tables from this document, the number of digits reported does not necessarily reflect the accuracy or precision of the calculation. In most tables, three to four digits after the decimal place have been retained, to prevent round-off errors in subsequent calculations.

Table 2 summarizes the reported characteristics of the N Reactor SNF. For most of the calculations, the composition of fresh (unirradiated) fuel was used. Use of the fresh fuel is conservative, since most fission products have significant neutron absorption cross sections, and the unirradiated fuel has a higher fissile content than partially spent fuel. For Case 9 (Table 8), the composition of Mark IA fuel 10 years since discharge with 16% of the Pu as ^{240}Pu, estimated using data from Table 3-8 in Reference 1 (Attachment III, spreadsheet "N-Reactor.xls", sheet "Burnup Fuel"), was used.

Table 1. Steel and Aluminum Alloy Compositions

Element	Aluminum 1100[a]		A516 Carbon Steel[b]		304L Stainless Steel[c]		316L Stainless Steel[d]	
	Weight %	Atom Fraction	Weight %	Atom Fraction	Weight %	Atom Fraction	Weight %	Atom Fraction
Al	99.00	0.9930						
C			0.30	0.0138	0.03	0.0014	0.03	0.0014
Mn			1.03	0.0103	2.00	0.0199	2.00	0.0202
P			0.04	0.0006	0.05	0.0008	0.05	0.0008
S			0.04	0.0006	0.03	0.0005	0.03	0.0005
Si	0.45	0.0043	0.28	0.0054	0.75	0.0146	0.75	0.0148
Cr					19.00	0.1997	17.00	0.1810
Cu	0.05	0.0002						
Ni					10.00	0.0931	12.00	0.1132
Mo							2.50	0.0144
N					0.10	0.0039	0.10	0.0040
Fe	0.50	0.0024	98.33	0.9694	68.05	0.6660	65.55	0.6498
Total	100.00	1.0000	100.00	1.0000	100.00	1.0000	100.00	1.0000

Sources: [a]Based on Al 1100 composition in Reference 61 (p. 7, Table 1)
[b]Reference 40 (p. 321, Table 1)
[c]Reference 47 (p. 2, Table 1)
[d]Reference 52 (p. 2, Table 1)

Table 2. N Reactor (U-metal) SNF Composition

Fuel Type	Mark IA Inner Rod (Fresh Fuel)[a]	Mark IA Outer Rod (Fresh Fuel)[a]	Mark IA Inner & Outer Rod (Decayed)[b]	Mark IV Inner & Outer Rod (Fresh Fuel)[a]
Isotope	**Weight %**	**Weight %**	**Weight %**	**Weight %**
U-234			0.0070	
U-235	0.9470	1.2500	0.7423	0.9470
U-236	0.0392	0.0392	0.1185	0.0392
U-238	99.0138	98.7108	98.8451	99.0138
Np-237			0.0204	
Pu-239			0.2210	
Pu-240			0.0440	
Pu-242			0.0016	
Sum	100	100	100	100

Sources: [a]Reference 1, Table 3-1
[b]Reference 1, Table 3-8; as calculated in Attachment III ("N-Reactor.xls"; sheet "Burnup Fuel"). This composition was used only for Case 9 (Table 8).

Table 3 gives the composition of the HLW glass used in the calculations (Ref. 31, Attachment I, p. I-7). The composition in Reference 31 was simplified to produce the values listed in Table 3 (worksheet "Composition" in spreadsheet "N-Reactor.xls" in Attachment III). Minor elements or elements with questionable thermodynamic data were removed (Ag, Cr, Cs, Cu, Li, Mn, Ni, Pb, Th, Ti, Zn), and shorter half-life Pu isotopes were "predecayed" to longer half-life U isotopes: ^{242}Pu was converted to ^{238}U; ^{241}Pu was converted to ^{237}Np, which was converted to ^{233}U; ^{240}Pu was converted to ^{236}U; ^{239}Pu was converted to ^{235}U; and ^{238}Pu was converted to ^{234}U. Since small amounts of neutron absorbers (Ag, Th, Zn) were removed in the simplified glass composition, this approach is conservative for internal criticality analyses. This simplification of the HLW glass composition allows the material to be entered as a pseudo-mineral, GlassSRL, in the EQ6 database, "data0.ymp" (Attachment III). If the HLW glass is entered in the database as a mineral, a pH dependent glass degradation rate using the EQ6 transition state theory (TST) formalism (Ref. 25, Section 3.3.3) can be applied.

Table 3. HLW Glass Composition[a] and Degradation Rate Constants

Element	Weight %	Moles/100g HLW Glass[b]
O	4.2605E+01	2.7039E+00
U	1.8612E+00	7.8186E-03
Ba	1.4718E-01	1.0751E-03
Al	2.3285E+00	8.6298E-02
S	1.2849E-01	4.0071E-03
Ca	6.5021E-01	1.6224E-02
P	1.5136E-02	4.8866E-04
Si	2.1808E+01	7.7649E-01
B	3.1486E+00	2.9124E-01
F	3.1565E-02	1.6615E-03
Fe	9.6172E+00	1.7221E-01
K	2.9347E+00	7.5059E-02
Mg	8.1001E-01	3.3327E-02
Na	1.3259E+01	5.7672E-01
Total	1.0000E+02	4.7465E+00
Total Rate Constant[c] = $k_1[H+]^{-0.4} + k_2[H+]^{0.6}$ (mol/cm^2·s)[d]		
Moderate Rate Constant (k_1)	(liter/cm^2·s)	8.85753E-19
High Rate Constant (k_1)	(liter/cm^2·s)	1.07560E-17
Moderate Rate Constant (k_2)	(liter/cm^2·s)	7.97555E-13
High Rate Constant (k_2)	(liter/cm^2·s)	4.87424E-12

Sources: [a]Simplified composition based on Reference 31 (Attachment II, p. II-7) as calculated in spreadsheet "N-Reactor.xls", sheet "Composition" (Attachment III)
[c]Reference 35; (Section 6.2.3.3, Equations 7 and 8); Attachment III ("N-Reactor.xls", sheet "Rates"). rates checked against Reference 28.

NOTES: [b]This is the composition added to "data0.ymp" for the pseudo-mineral, GlassSRL.
[d]One mole = 100g HLW glass. The molecular weight of all WP components was set to 100 g to simplify inputs to EQ6.

As was shown in Sections 5.3.2 and 5.3.3 of Reference 32, EQ6 estimates of U loss, from the WP, are not greatly affected by substantial variations in the composition of the HLW glass. The actual HLW glass composition used in the GPCs may vary significantly from these values, since the sources of the HLW glass and melting processes are not currently fixed. For example, compositions proposed for Savannah River Site HLW glass vary by a factor of ~6 in U_3O_8 content, from 0.53 to 3.16 weight percent (Ref. 33, p. 3.3-15, Table 3.3.8.). The Si and alkali metal contents (Na, Li, and K) of the HLW glass have perhaps the most significant bearing on EQ6 calculations. The amount of Si in the HLW glass strongly controls the amount of clay that forms in the WP, and the Si activity controls the presence of insoluble uranium phases such as soddyite [$(UO_2)_2SiO_4 \cdot 2H_2O$], sodium boltwoodite ($NaUO_2SiO_3OH \cdot 1.5H_2O$), or α-uranophane [$Ca(UO_2SiO_3OH)_2 \cdot 5H_2O$]. As the HLW glass degrades in an EQ6 run, the alkali metal content of the corrosion products increases and the pH rises. The Si and alkali metal contents in Table 3 are typical for proposed DOE HLW glasses (Ref. 31).

A pH-dependent rate for HLW glass degradation was derived from Reference 35 (Sec. 6.2.3.3, Eq. 7 and 8), and normalized in spreadsheet "N-Reactor.xls", sheet "Rates" (Attachment III). The first rate mechanism (described with k_1) in Table 3 is dominant at pH values above 7, while the second rate mechanism (described with k_2) is dominant at pH values below 7. The high glass degradation rate constants in Table 3 are those predicted at 50°C, while the moderate rate constants are those derived for degradation at 25°C (Ref. 35, Sec. 6.2.3.3, Eq. 7 and 8).

Table 4 provides molar volume, density, initial moles, reaction rate constants, and surface area for all of the materials in the N Reactor codisposal WP that were considered in the calculation. These values were calculated using volarea (Attachment III) with the geometries of the waste package components. The molar volume is the molecular weight divided by the density. For each EQ6 special reactant, the molecular weight is assumed to be 100 g/mol, which makes the calculation less complicated and has no effect on the results. The initial moles and the surface area in Table 4 are divided by the total initial void volume of 4268.479 liters to obtain normalized values based on one liter of water which is used by the EQ6 code. The details of the void volume calculation are provided in spreadsheet "N-Reactor.xls" sheet "Void_calc" (Attachment III).

Total uranium in the waste package can be obtained by adding the U in the HLW glass to the U present in the fuel. To calculate total uranium for the Mark IA and Mark IV fuel, moles from Table 4 are converted to Kg by multiplying by the initial void volume (4268.479L) and the molecular weight (100g/mole for special reactants) to obtain the Kg of U in the fuel for two MCO stands. These values were then compared to those from reference 1 (section 3.1.2) and found to be only 0.46% different. Unlike the fuel which is 100% U, the glass is only 0.78% U. To obtain the U in the glass, the moles of glass (Table 4) must be multiplied by 0.0078 to obtain the moles of U. This is then multiplied by the void volume (4268.479 L), molecular weight of U (238 g/mole), and divided by 1000 to obtain Kg of U in the glass. Total U for waste packages containing Mark IA Fuel and Mark IV Fuel is 9711.6 Kg and 12,847.6 Kg respectively

Table 4. Properties of Materials in the N Reactor SNF Codisposal WP

EQ6 Reactant Name	WP Component	V[a] Molar Volume (cm^3/mol)	Density (g/cm^3)	Initial Kg	m_I[b] Initial Moles	rk[c] Rate Constant ($mol/cm^2 \cdot s$) 1	rk[c] Rate Constant ($mol/cm^2 \cdot s$) 2	sk[d] Surface Area (cm^2)
GlassSRL	HLW Glass	35.09	2.85[e]	5,767	13.51	(Table 3)	(Table 3)	729.5
MarkIA_fuel_out	Mark IA Fuel (outer rods)	5.313	18.82[f]	3,227	14.95	2.0255E-9[g]	Not Applicable (N/A)	233.3
MarkIA_fuel_in	Mark IA Fuel (inner rods)	5.313	18.82[f]	6,381	7.559	2.0255E-9[g]	N/A	93.03
MarkIV_fuel	Mark IV Fuel (inner and outer rods)	5.313	18.82[f]	12,745	29.86	2.0255E-9[g]	N/A	384.1
MarkIA_out_burnup	Mark IA Fuel (outer rods - decayed)	5.313	18.82[f]	6,351	14.88	2.0255E-9[g]	N/A	232.2
MarkIA_in_burnup	Mark IA Fuel (inner rods - decayed)	5.313	18.82[f]	3,211	7.522	2.0255E-9[g]	N/A	92.57
MCOMain_304L_MarkIA	MCO canister and baskets	12.59	7.94[h]	3,781	8.857	2.516E-14[i]	8.656E-12[j]	124.2
MCOMain_304L_MarkIV	MCO canister and baskets	12.59	7.94[h]	2,700	6.326	2.516E-14[i]	8.656E-12[j]	114.1
MCOTop_304L	MCO top	12.59	7.94[h]	2,985	6.995	2.516E-14[i]	8.656E-12[j]	8.523
GPC_304L	GPCs	12.59	7.94[h]	1,483	3.475	2.516E-14[i]	8.656E-12[j]	82.06
APlate_A516	A plates and MCO stands	12.74	7.85[k]	1,223	2.867	1.798E-11[l]	N/A	78.33
Liner_316NG	EDA II Liner	12.53	7.98[h]	13,189	30.90	2.529E-14[l]	5.056E-13[j]	63.06
Al_1100_MarkIA	Al spacers	36.90	2.71[h]	91.2	0.2137	2.536E-13[l]	N/A	35.29
Al_1100_MarkIV	Al spacers	36.90	2.71[h]	80.7	0.1890	2.536E-13[l]	N/A	33.22

NOTES: [a] ***V*** equals the molecular weight (The molecular weight of all WP components was set to 100g/mol to simplify inputs to EQ6) divided by the density (g/cm^3).
[b] m_I equals initial mass (g) divided by 100 g/mol divided by 4268.479 liters void volume in the WP.
[c] ***rk*** equals the reaction rate ($g/cm^2 \cdot s$) divided by 100 g/mol. These rate constants must be multiplied by the normalized surface area (***sk***) in cm^2 of each WP component to calculate the actual degradation rate in 100-g mol/s of that component.
[d] ***sk*** equals total surface area divided by 4268.479 liters of void volume in the WP.

Sources: [e] Based on a range of HLW glass densities in Reference 62 (p. 26 Fig. 2 and pp 54-57)
[f] Reference 1 (Sec. 3.1.4, p. 22)
[g] Reference 36, Section 6.3.7, Table 1 estimates an expected degradation rate of 175,000 $mg/m^2 \cdot d$ which is converted to 100g-$mol/cm^2 \cdot s$ in "N-Reactor.xls", sheet "Rates" (Attachment III).
[h] Reference 60 (p. 7, Table XI)
[i] This rate constant was converted to ***rk*** in 100g-$mol/cm^2 \cdot s$ from a corrosion rate of 0.1 μm/year (Ref. 49, pp. 11-13) in "N-Reactor.xls", sheet "Rates" (Attachment III).
[j] Rates were calculated in spreadsheet "N-Reactor.xls", "Rates" sheet (Attachment III) using Eq. 3-14 derived from Fig. 3-15 (Reference 30, Sec. 3.1.5.4.1).
[k] Reference 59 (p. 9)
[l] Values from Reference 29 (p. 2.2-96 through P2.2-98) were used to derive a corrosion rate of 72 μm/year in spreadsheet "A516_Rate.xls",sheets "Prob" and "Prob_Chart" (Attachment III). This rate as well as rate from Ref. 38 (p603) was converted to ***rk*** in 100g-$mol/cm^2 \cdot s$ in "N-Reactor.xls", sheet "Rates" (Attachment III).

The degradation rates in Table 4 are average or high degradation rates (indicated by "1" or "2"). The true reaction rate is obtained by multiplying ***rk*** by ***sk*** to get mol/s. Inspection of the rates shows that for a comparable surface area, the A516 carbon steel is expected to degrade much more rapidly than the stainless steels (316L and 304L).

The A-plates are composed of A516 carbon steel, and serve two purposes: they center and hold in place and separate the MCOs and GPCs; and prevent them from transmitting undue stress to each other in the event of a fall (tip-over) of the entire WP. The MCO stands are also constructed of A516. In a breach scenario, these A516 WP components will be exposed to water and corrosion before the rest of the WP, and are expected to degrade within a few hundred to a few thousand years. Precipitation of hematite (Fe_2O_3) or goethite (FeOOH) will result from the oxidation of iron in the A516 (Ref. 2).

5.1.1.2 Chemical Composition of J-13 Well Water

It was assumed that the water composition entering the WP would be the same as that for water from well J-13 (Assumptions 3.2 and 3.3). This water has been analyzed repeatedly over a span of at least 20 years (Ref. 54, DTN: MO0006J13WTRCM.000; Ref. 6, Table 4.2. The composition of J-13 well water as used in this calculation has been adjusted slightly (see assumptions 3.9 and 3.13). Tables 5 and 6 contain the EQ3NR input file constraints for J-13 well water composition and the EQ6 input file elemental molal composition for J-13 well water used for this calculation.

The "Basis Species" column of Table 5 lists the chemical species names recognized by EQ3NR and EQ6. Since some of the components of J-13 well water, as analyzed (Ref. 54, DTN: MO0006J13WTRCM.000 and Ref. 6, table 4.2, are in a different chemical form than the species listed in this column, these components must be substituted or "switched" with the basis species for input into EQ6 and are listed in the "Basis Switch" column. Basis species listed as "Trace" in the "Basis Switch" column are not found in J-13 well water, as analyzed (Ref. 54, and Ref. 6), but are in the composition of other WP components and must be input at a minimum concentration for numerical stability in EQ6 calculations.

Table 5. EQ3NR Input File Constraints for J-13 Well Water Composition

Basis Species	Basis Switch	Concentration	Units
redox		-0.7	log fO_2
Na+		4.580E+01[c]	mg/L
SiO_2(aq)		6.097E+01[c]	mg/L
Ca++		1.300E+01[c]	mg/L
K+		5.040E+00[c]	mg/L
Mg++		2.010E+00[c]	mg/L
Li+		4.800E-02[d]	mg/L
H+		8.1[c]	pH
HCO_3-	CO_2(g)	-3[c]	log fCO_2
O_2(aq)		5.600E+00	mg/L
F-		2.180E+00[c]	mg/L
Cl-		7.140E+00[c]	mg/L
NO_3-	NH_3(aq)	8.780E+00[c]	mg/L
SO_4--		1.840E+01[d]	mg/L
$B(OH)_3$(aq)		7.660E-01[d]	mg/L
Al+++	Diaspore	0	Mineral
Mn++	Pyrolusite	0	Mineral
Fe++	Goethite	0	Mineral
HPO_4--		1.210E-01[d]	mg/L
Ba++	Trace	1.000E-16	Molality[a]
CrO_4--	Trace	1.000E-16	Molality[a]
Cu++	Trace	1.000E-16	Molality[a]
MoO_4--	Trace	1.000E-16	Molality[a]
Ni++	Trace	1.000E-16	Molality[a]
Np++++[b]	Trace	1.000E-16	Molality[a]
Pu++++[b]	Trace	1.000E-16	Molality[a]
UO_2++	Trace	1.000E-16	Molality[a]

NOTES: [a]A trace concentration (1.0E-16 molal) is added for elements that are not in J-13 well water as analyzed, but are in the composition of the WP components, to ensure numerical stability in EQ3/6 runs.
[b]Only included for Case 9 in Table 8.

Sources: [c]Ref. 54 (DTN: MO0006j13WTRCM.000)
[d]Ref. 6, Table 4.2

Table 6. EQ6 Input File Elemental Molal Composition for J-13 Well Water

Element	Mole/kg	Element	Mole/kg
O	5.55E+01	Mg	8.27E-05[a]
Al	2.55E-08	Mn	3.05E-16
B	1.24E-05	Mo	1.00E-16
Ba	1.00E-16	N	1.42E-04[a]
Ca	3.24E-04[a]	Na	1.99E-03[a]
Cl	2.01E-04[a]	Ni	1.00E-16
Cr	1.00E-16	S	1.92E-04[a]
Cu	1.00E-16	Si	1.02E-03[a]
F	1.15E-04[a]	U	1.00E-16
Fe	3.60E-12	K	1.29E-04[a]
H	1.11E+02	Li	6.92E-06
Np	1.00E-16	C	2.09E-03[a]
Pu	1.00E-16	P	1.26E-06

Sources: [a]Ref. 54 (DTN:MO0006J13WTRCM.000)
Ref. 6, Table 4.2

5.1.1.3 Drip Rate of J-13 Well Water into a WP

It is assumed (Assumption 3.14) that the drip rate onto a WP is the same as the rate at which water flows through the WP. The drip rate is taken from a correlation between percolation rate and drip rate (Ref. 39, Tables 2-55 and 2-56). Specifically, percolation rates of 40 mm/year and 8 mm/year correlate with drip rates onto the WP of 0.15 m^3/year and 0.015 m^3/year, respectively. The choice of these particular percolation and drip rates is discussed in detail in Reference 27 (Section 5.1.1.3, p. 19).

For the present study, the range of allowed drip rates included an upper value of 0.015 m^3/yr and a lower value of 0.0015 m^3/yr. The upper value corresponds to the mean value for the percolation rate of 8 mm/year (Ref. 39, Figure 2.3-108), and the lower value is simply $1/10^{th}$ of the upper value.

5.1.1.4 Densities and Molecular Weights of Solids

For input to criticality calculations, one must convert moles of solids to volume of solids. A few solid phases contribute the overwhelming bulk of the total volume; Table 7 provides some of the densities and molar volumes for these phases. The EQ6 database used for this calculation ("data0.ymp", Attachment III) did not contain molar volumes for some of the solids that were predicted to form during the EQ6 runs for the cases in Table 8. Molar volumes for these solids were calculated from the molecular weights of the solids in "data0.ymp" and the solid densities from various sources, as noted in Table 7. The current version of EQ6 (Section 4) performs the volume calculations for each element automatically.

Table 7. Densities, Molecular Weights and Molar Volumes of Precipitated Solids

Solid	Density (kg/m^3)	Molecular Weight (g/mole) [c]	Molar Volume (cm^3/mol) [c]	Calculated Density (g/cm^3) [f]
Gibbsite [$Al(OH)_3$]		78.004	31.956	2.441
Hematite (Fe_2O_3)	5260[a]	159.688	30.274	5.275
Pyrolusite (MnO_2)	5060[a]	86.937	17.181	5.060[a]
Goethite (FeOOH)		88.852	20.820	4.268
Trevorite ($NiFe_2O_4$)	5165[a]	234.382	45.379[e]	5.165[a]
Nontronite-Ca		424.293	131.100	3.236
Nontronite-K		430.583	135.270	3.183
Nontronite-Mg		421.691	129.760	3.250
Nontronite-Na		425.267	132.110	3.219
Fluorapatite [$Ca_5(PO_4)_3F$]	3200[a]	504.302	157.594[g]	3.2[a]
Hydroxylapatite [$Ca_5(PO_4)_3OH$]	3080[a]	502.311	163.088[g]	3.08[a]
Mesolite	2259[a]	387.783	171.661[g]	2.259[a]
$Ni_3(PO_4)_2$	4396[b]	366.023	83.263[g]	4.396[b]
α-Uranophane [$Ca(UO_2SiO_3OH)_2 \cdot 5H_2O$]	3830[a]	856.392	223.601[g]	3.83[a]
$(UO_2)_3(PO4)_2 \cdot 6H_2O$	3500[b]	1108.118	316.605[g]	3.5[b]
$Na_4UO_2(CO_3)_3$	3630[b]	542.013	149.305[g]	3.63[b]
$CaUO_4$	7459[b]	342.105	45.865[g]	7.459[b]
NpO_2	11110[d]	268.999	24.220	11.11[d]
PuO_2	11.581[e]	275.999	23.830	11.581[e]

Sources: [a]Reference 42, pp. 289 (fluorapatite), 356 (hematite), 389 (hydroxylapatite), 547 (mesolite), 704 (pyrolusite), 880 (trevorite), and 903 (α-uranophane).
[b]Reference 56, JCPDS cards for $Ni_3(PO4)_2$ (38-1473), $(UO_2)_3(PO4)_2 \cdot 6H_2O$ (30-1405), $CaUO_4$ (44-583), $Na_4UO_2(CO_3)_3$ (11-81).
[c]Attachment III (EQ3/6 Data base, "data0.ymp") unless otherwise noted.
[d]Reference 55, (p. B101).
[e]Reference 57, (p.C-103).

NOTES: [f]Calculated from the molecular weight and molar volume unless other wise noted.
[g]Calculated from the molecular weight and density.

5.1.1.5 Atomic Weights

Atomic weights were taken from References 43 and 44 (Chart of the Nuclides), and are listed in spreadsheet "N-Reactor.xls" sheet "Atomic Weights_New" (Attachment III).

5.2 DATA CONVERSION

The data presented in Section 5.1 are not in a form suitable for entry into EQ3/6. The transformation to EQ3/6 format involves converting mass fractions to mole fractions; normalizing surface areas, volumes, and moles to 1 liter reactive water in the system; and

converting rates to $mol/cm^2 \cdot s$. Most of these conversions are straightforward and are performed in the spreadsheets that are included in the attached CD for this document (Attachment III). Reference 27 (Section 4) describes the conversion process in detail.

5.3 EQ6 CALCULATIONS AND SCENARIOS REPRESENTED

The rationale for selection of scenarios in EQ6 simulations is to provide conservative criticality assessments of solubility and transport of fissile materials (i.e., U, Pu, or Np compounds) in the WP. An internal criticality is possible if the fissile material remains behind in the WP. Soluble U, Pu, and Np carbonate complexes will form in the high pH solutions produced when the HLW glass degrades.

The "*Disposal Criticality Analysis Methodology Topical Report*" document defines the internal and external degradation scenarios for disposal criticality analysis (Ref. 46, pp. 3-9 through 3-12). The internal degradation configurations are based on the assumption that groundwater drips onto the upper surface of the WP and penetrates it. Groundwater accumulates inside the WP, which could dissolve and flush the SNF from the WP. Following is a summary of three groups of degradation configurations from Reference 46:

1. WP internals degrade faster than the waste forms
2. WP internals degrade at the same rate as the waste form
3. WP internals degrade slower than the waste forms.

The WP internals include all components within the WP, except SNF. The waste forms refer to SNF. The above configurations set the framework in which EQ6 scenarios could be developed. The scenarios are based on a sequence of chemical reactions as a function of time and can be divided into two general categories: single stage cases and two-stage cases.

Single-Stage Cases–In these calculations, all WP internals, including SNF, come in contact with groundwater simultaneously. These cases correspond to an extreme in which the zirconium cladding is breached immediately, thereby exposing all or a portion of the spent fuel as soon as the WP corrosion barriers are breached. These cases result in the highest dissolved radionuclide levels, and might provide the most conservative estimate of fissile material loss.

Two-Stage Cases–These EQ6 calculations start with the breach of the WP allowing groundwater to come in contact with WP internals outside the MCOs ("stage A"); during this stage the MCOs remain intact. The second stage ("stage B") starts with breach of the MCOs and interaction of groundwater with material inside the MCOs, as well as waste forms and unaltered reactants remaining from stage A. These cases were designed to produce the lowest possible pH, by first exposing the HLW glass to J-13 well water to remove alkalinity, prior to exposure of the SNF in the second stage.

In total, 10 cases of single- and two-stage EQ6 simulations with different steel and HLW glass degradation rates, as well as varied water fluxes through the WP, were run. These cases are discussed in the following sections.

5.3.1 EQ6 Run Conditions and Nomenclature

The EQ6 codes were used to run the 10 cases summarized in Table 8. In general each case could be classified as single- or two-stage. Cases 1-9 are single-stage, and involve simultaneous exposure of the SNF and the WP materials to J-13 well water. Considering that the SNF rods are within zirconium cladding, for a conservative approach, it was assumed (Assumption 3.20) that cladding is fully breached immediately after contact with water.

The "File Names" column in Table 8 gives the root file names used to describe the runs. The EQ6 input files corresponding to these runs end with the extension ".6i" (e.g., "N40h1112.6i" is an EQ6 input file name for Case 3); these input files are included in the attached CD accompanying this calculation (Attachment III). Each EQ6 run has associated tab-delimited text files, also included in the attached CD (e.g., "N40h1112.elem_aqu.txt" for Case 3). The text files list total moles of elements in the aqueous phase ("?.elem_aqu.txt"), total moles of each element precipitated as minerals ("?.elem_min.txt"), and total moles of each element ("?.elem_tot.txt"), which is the sum of moles in the aqueous and mineral phases plus the unreacted, or remaining moles of reactants (WP components). Since the HLW glass WP component was entered into the "data0.ymp" file as a pseudo-mineral for this calculation, the remaining moles of this reactant were not included in the "?.elem_tot.txt" files. Several input files, corresponding to separate EQ6 runs, may be grouped into a "Case". Most of the important run conditions could be inferred from the root file name. Evaluation of root file names for most cases from left to right is as follows:

The first letter "N" corresponds to N Reactor SNF.

The second character (first digit after "N") is "4" for cases with Mark IV N Reactor SNF or "1" for cases with Mark IA N Reactor SNF.

The third character (second digit after "N") corresponds to revision or continuation of input file for the single- and two-stage cases; for each case, the numbers range from 0 to 2. Runs that do not converge usually require removal of the exhausted reactants and restart of the run.

The fourth character (third digit after "N") in the two-stage runs are "A" for the first stage or "B" for the second stage of the run.

The fourth character in the single-stage cases corresponds to special run conditions which are defined in the note beneath Table 8.

The fifth digit is 1 or 2 corresponding to the average or high rates of steel corrosion in Table 4.

The sixth digit in this block is 1, 2, or 0, with 1 and 2 corresponding to the moderate and high glass corrosion rates listed in Table 3; and 0 corresponding to no HLW glass present in the EQ6 run.

The seventh digit in the block is 1 or 0, with 1 corresponding to SNF dissolution rate in Table 4, and 0 corresponding to no SNF present in the EQ6 run.

The last digit in the block encodes the choice of drip rate, with 1 and 2 corresponding to 0.0015 m^3/year and 0.015 m^3/year, respectively.

5.3.2 Examination of Cases

Table 8 summarizes all the cases run, as well as the total percentage of U (plus Pu and Np for Case 9) loss at the end of the EQ6 runs. These losses were calculated in the spreadsheet "Nreactor_U.xls", sheet "U-losses" (Attachment III). The complete output tables (aqueous, mineral, and total moles) for all the cases are included in the attached CD, as text files (Attachment III). A summary of the files included in the attached CD is given in Attachment II.

The losses calculated above were then checked by hand calculations of the areas beneath the U curve on Figures 1 through 23. These calculations produced numbers close to those calculated in the spreadsheet "Nreactor_U.xls" confirming that the % loss of U from the waste packages is very low and the numbers presented are correct. Case 5 is used as an example of how this hand calculation was executed –Attachment III, "Nreactor_U.xls" sheet "check"

Tables 9 through 27 illustrate the limits of system behavior for the single-stage runs. Single stage runs show U (plus Pu and Np for Case 9) loss from the SNF and HLW glass to alteration products and solution as a function of reaction time, and how each output varies depending upon input steel corrosion rates, HLW glass corrosion rates, SNF corrosion rates, and fluid flow rates. The two-stage run (Case 10) provides information on how the system might behave under a number of extreme scenarios. Examination of the results in Table 8 reveals the following generalizations about U (plus Pu and Np for Case 9) release from the WP.

1. Predicted total losses of U from the WP were less than 2% for all of the cases shown in Table 8. Uranium loss can be attributed to the formation of four major minerals including Schoepite [UO_3:$2H_2O$], Sodium Boltwoodite [$NaUO_2SiO_3OH$:$1.5H_2O$], $(UO_2)_3(PO_4)_2$:$6H_2O$, and α-Uranophane [$Ca(UO_2SiO_3OH)_2$:$5H_2O$] with Schoepite being the most dominant.

2. Case 10, the two-stage run, predicted that all of the U in the HLW glass (1.10% of the total U in the WP) would be lost from the WP for conditions of average steel, high HLW glass degradation rates and low drip rate simulated by the first stage of the run. Only 0.02% of the total U in the WP (from Mark IA SNF only) was predicted to be lost during

the conditions simulated by the second stage of Case 10, with low steel, average SNF degradation rates, and low drip rate.

3. Cases 2 and 5 had predicted total U losses from the WP of close to 1%. Both these cases simulated conditions of high steel, average fuel, and low glass degradation rates, with a low drip rate.

4. Predicted loss of U from the WP was very low (0-0.16%) for the rest of the Cases shown in Table 8.

5. Case 9 was run assuming a decayed composition for N Reactor Mark IA SNF (Table 2). Although predicted total loss of U was very low for this case (0.02%), predicted total loss of Np was high (~83%) and predicted total loss of Pu was low (<2%).

Table 8. Summary of Cases Run, Associated Input File Names, Percent Fuel Surface Exposed to Corrosion, Percent U Loss, and Fe Oxide Corrosion Product

Case	File Names[b]	% Fuel Surface Area	Mark IV SNF	Mark IA SNF	% U Loss[a]	% Np Loss[a]	% Pu Loss[a]
1	N40h1111	100	√		0.03	N.A.[c]	N.A.
2	N40h2111	100	√		0.75	N.A.	N.A.
3	N40h1112	100	√		0.12	N.A.	N.A.
4	N10h1111	100		√	0.02	N.A.	N.A.
5	N10h2111	100		√	0.98	N.A.	N.A.
6	N10h1112	100		√	0.16	N.A.	N.A.
7	N10#1111	10		√	0.02	N.A.	N.A.
8	N10&1111	0		√	0.00	N.A.	N.A.
9[d]	N10h1211	100		√	0.02	82.81	1.58
10	N10A1201	0		√	1.10	N.A.	N.A.
	N10B1011	100			0.02	N.A.	N.A.

NOTES: [a] U, Pu and Np losses are a percentage of total moles of U, Pu and Np in SNF and HLW glass. Pu and Np are only relevant to case 9, because the other cases use only fresh fuel.
[b] Explanation of special symbols in root file names:
note: hematite was not suppressed in any of the EQ6 runs.
h = normal run without any special conditions applied
# = 100% fuel moles and 10% fuel surface area exposed to corrosion
& = 100% fuel moles and 0% fuel surface area exposed to corrosion
A = First stage of a two-stage run
B = Second stage of a two-stage run
[c] Not Applicable (fresh fuel contains no Pu or Np)
[d] Case 9 was run with the decayed fuel compositions in Table 2.

Table 9. Predicted Elemental Composition of Corrosion Products (kg), Total Mass (kg) and Density in Selected Years for Case 1 (n40h1111)

Years	2354	112760	634010
Element			
O	4.932E+03	7.221E+03	1.195E+04
Al	2.784E-01	1.216E+01	6.449E+01
B	1.993E-14	6.389E-14	0.000E+00
Ba	1.760E-02	7.705E-01	4.103E+00
Ca	1.293E-01	4.859E+00	2.753E+01
Cl	0.000E+00	0.000E+00	2.150E-13
Cr	0.000E+00	2.917E-01	1.553E+00
Cu	1.876E+02	1.806E+02	1.695E+02
F	0.000E+00	0.000E+00	5.181E-13
Fe	1.349E+03	5.904E+03	1.417E+04
H	2.159E+02	2.188E+02	2.313E+02
C	0.000E+00	0.000E+00	6.315E-12
P	5.267E-01	3.635E+00	9.535E+00
K	5.942E-02	3.433E+00	1.968E+01
Li	0.000E+00	0.000E+00	1.781E-15
Mg	9.672E-02	3.968E+00	2.137E+01
Mn	1.706E+01	1.514E+02	3.969E+02
Mo	3.095E-01	1.163E+01	6.240E+01
N	0.000E+00	0.000E+00	9.702E-14
Na	1.939E-02	8.347E-01	7.262E+00
Ni	0.000E+00	3.825E+01	4.129E+02
S	4.110E-03	0.000E+00	1.943E-11
Si	8.096E+00	1.795E+02	8.068E+02
U	1.275E+04	1.275E+04	1.279E+04
Total (kg)	1.946E+04	2.669E+04	4.115E+04
Density (g/cm^3)	4.921	4.929	4.848

Table 10. Predicted Solution Elemental Composition (mole kg^{-1}) and pH in Selected Years for Case 1 (n40h1111)

Years	2354	112760	634010
pH	5.54	5.87	6.68
Element			
Al	1.716E-10	1.177E-11	2.089E-14
B	5.617E-03	8.359E-03	9.416E-03
Ba	5.050E-07	5.961E-07	3.387E-07
Ca	1.525E-04	6.426E-05	9.171E-05
Cl	2.014E-04	2.014E-04	2.014E-04
Cr	1.223E-01	5.382E-02	7.026E-03
Cu	1.164E-03	2.338E-04	3.729E-06
F	1.475E-04	1.635E-04	1.696E-04
Fe	9.707E-12	5.720E-12	1.691E-12
C	3.130E-05	4.781E-05	1.199E-04
P	1.687E-08	2.906E-08	1.282E-07
K	1.277E-03	1.776E-03	1.173E-03
Li	3.918E-06	6.915E-06	6.915E-06
Mg	8.200E-05	1.265E-04	5.256E-05
Mn	1.584E-10	3.231E-11	4.857E-13
Mo	1.577E-03	3.007E-03	8.157E-04
N	2.592E-03	1.301E-03	2.796E-04
Na	1.291E-02	1.838E-02	1.236E-02
Ni	6.124E-02	2.423E-02	3.626E-04
S	2.473E-03	4.582E-04	3.388E-04
Si	1.493E-04	1.856E-04	1.859E-04
U	1.771E-05	9.097E-06	8.808E-06

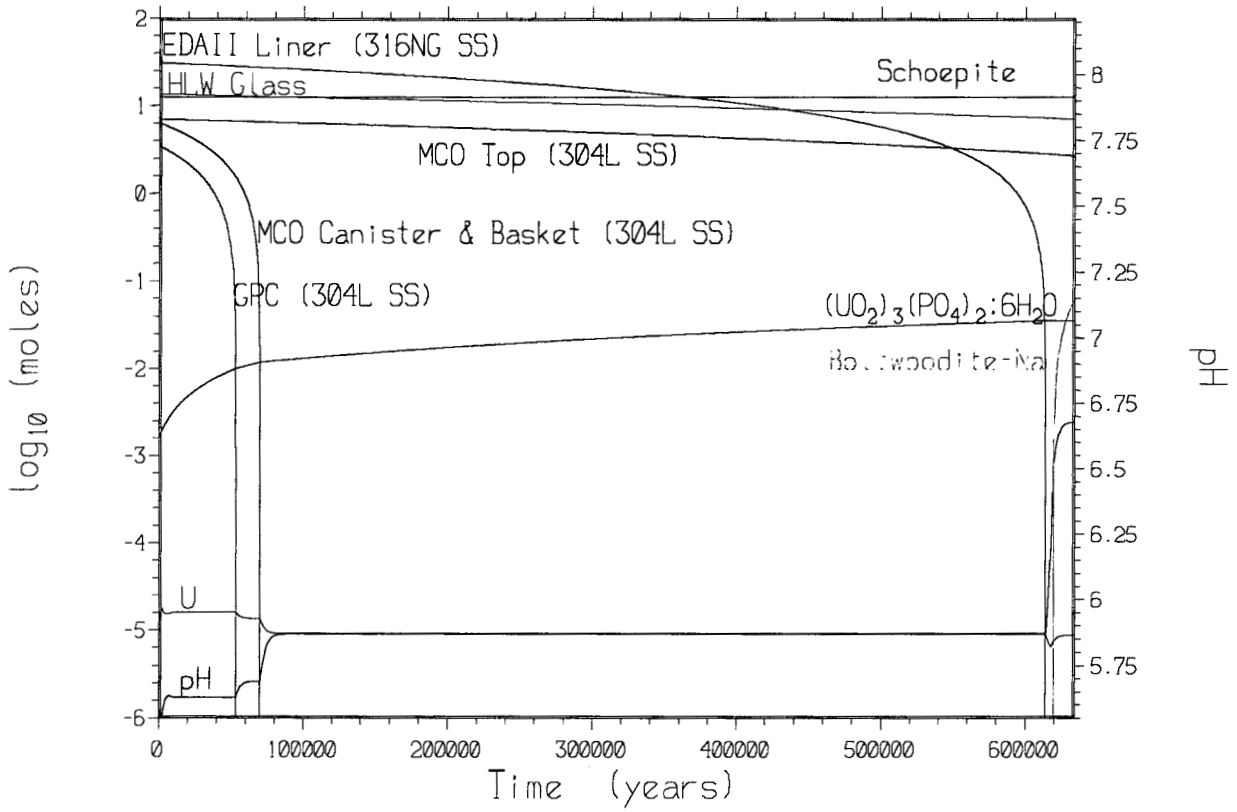

Figure 1. Predicted Concentration of Major Waste Package Components, Precipitated U Minerals, Total U in Solution, and pH as a Function of Time During Case 1 (n40h1111)

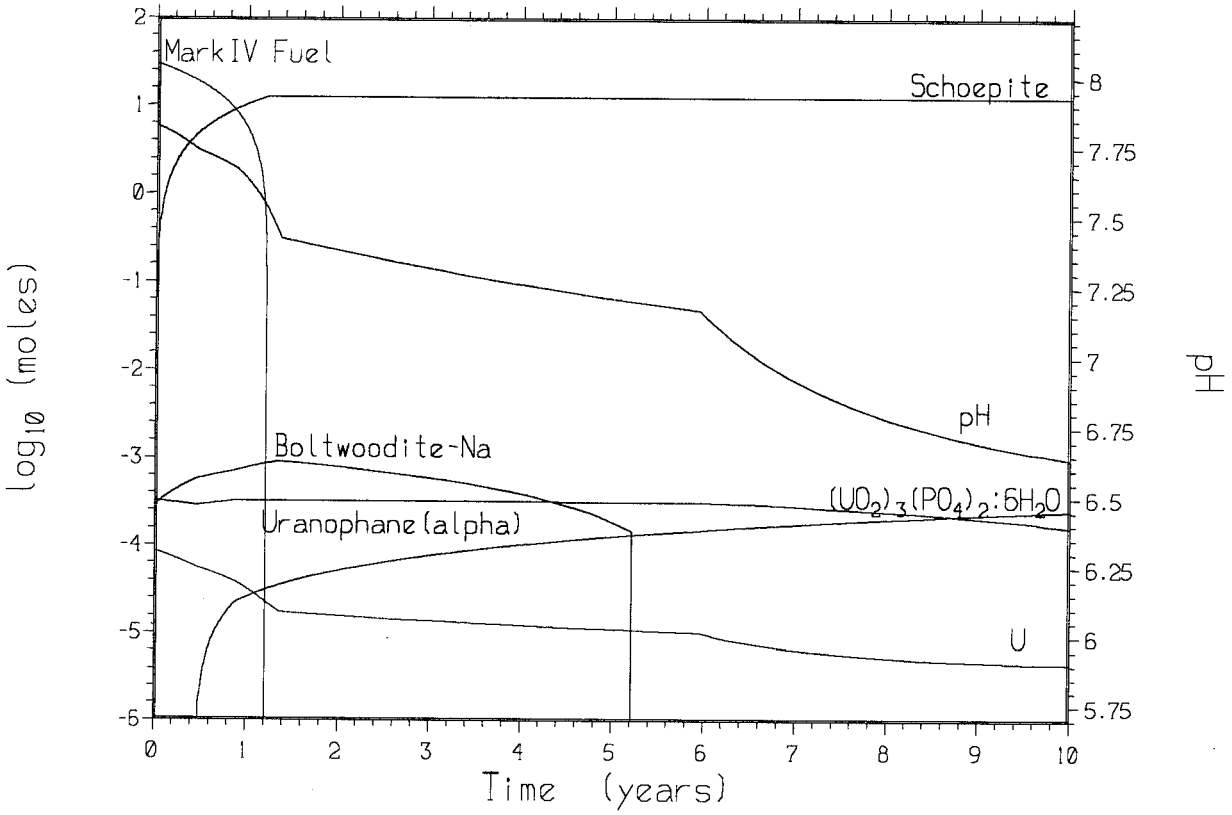

Figure 2. Predicted Concentration of N-Reactor SNF, Precipitated U Minerals, Total U in Solution, and pH as a Function of Time Early in Case 1(n40h1111)

Table 11. Predicted Elemental Composition of Corrosion Products (kg), Total Mass (kg) and Density in Selected Years for Case 2 (n40h2111)

Years	153	106000	634260
Element			
O	5.898E+03	1.151E+04	1.345E+04
Al	9.856E-02	2.127E+01	1.343E+02
Ba	5.794E-03	1.366E+00	8.696E+00
Ca	7.518E-02	7.889E+00	4.945E+01
Cl	4.343E-11	1.231E-17	0.000E+00
Cr	1.601E-05	9.749E-25	2.189E-29
Cu	6.081E+00	1.364E+02	1.364E+02
F	8.017E-11	3.957E-17	2.086E+00
Fe	3.723E+03	1.478E+04	1.525E+04
H	2.061E+02	2.217E+02	2.393E+02
C	3.467E-12	1.195E-01	7.605E-01
P	2.097E+00	9.726E+00	1.020E+01
K	1.561E-12	1.268E+01	3.485E+01
Mg	1.575E-11	6.532E+00	4.134E+01
Mn	8.690E+01	4.199E+02	4.199E+02
Mo	1.800E-01	0.000E+00	9.086E-29
N	2.057E-08	0.000E+00	0.000E+00
Na	7.678E-12	7.951E+01	7.225E+02
Ni	7.884E-08	9.881E+01	9.879E+01
S	1.024E+00	1.380E-15	0.000E+00
Si	3.255E+01	3.922E+02	1.472E+03
U	1.274E+04	1.276E+04	1.276E+04
Total (kg)	2.269E+04	4.046E+04	4.482E+04
Density (g/cm^3)	5.000	4.964	4.680

Table 12. Predicted Solution Elemental Composition (mole kg^{-1}) and pH in Selected Years for Case 2 (n40h2111)

Years	153	106000	634260
pH	3.74	7.87	8.21
Element			
Al	3.500E-06	8.884E-16	1.038E-07
B	2.855E-03	2.401E-02	1.239E-05
Ba	1.035E-06	1.681E-08	3.687E-09
Ca	5.316E-05	9.523E-07	5.610E-06
Cl	2.014E-04	2.014E-04	2.014E-04
Cr	3.084E+00	3.593E-13	1.000E-16
Cu	1.229E-01	8.864E-08	7.478E-08
F	1.313E-04	2.548E-04	1.147E-04
Fe	3.197E-10	1.131E-12	1.138E-12
C	2.437E-06	1.343E-03	3.752E-03
P	1.218E-08	6.676E-06	1.156E-06
K	8.629E-04	2.710E-03	2.522E-03
Li	3.610E-07	6.915E-06	6.915E-06
Mg	4.077E-04	2.870E-04	2.362E-04
Mn	1.126E-07	1.702E-15	5.594E-16
Mo	3.465E-03	1.981E-09	1.000E-16
N	6.051E-02	1.416E-04	1.416E-04
Na	7.621E-03	7.467E-04	1.829E-03
Ni	1.446E+00	1.181E-06	2.601E-07
S	3.802E-03	5.211E-04	1.915E-04
Si	7.666E-05	1.893E-04	3.689E-05
U	7.802E-03	1.026E-04	5.085E-04

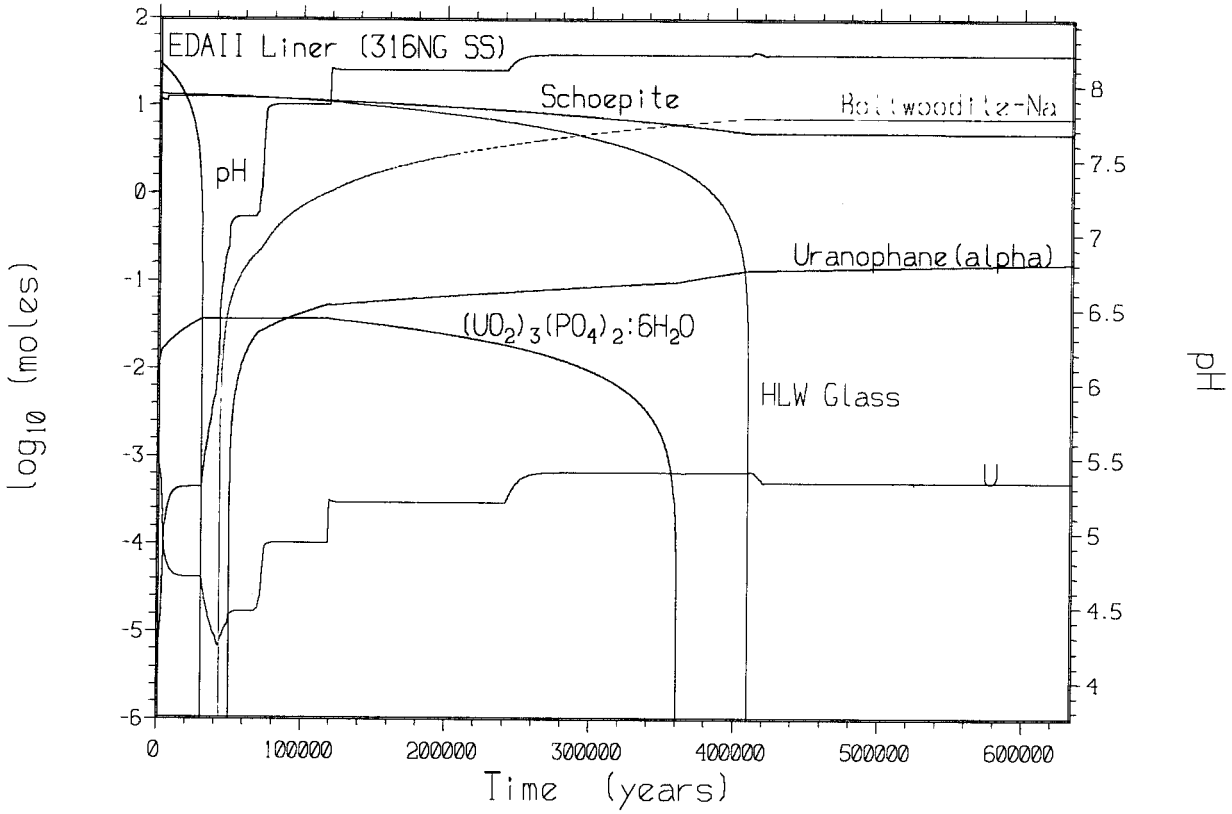

Figure 3. Predicted Concentration of Major Waste Package Components, Precipitated U Minerals, Total U in Solution, and pH as a Function of Time During Case 2 (n40h2111)

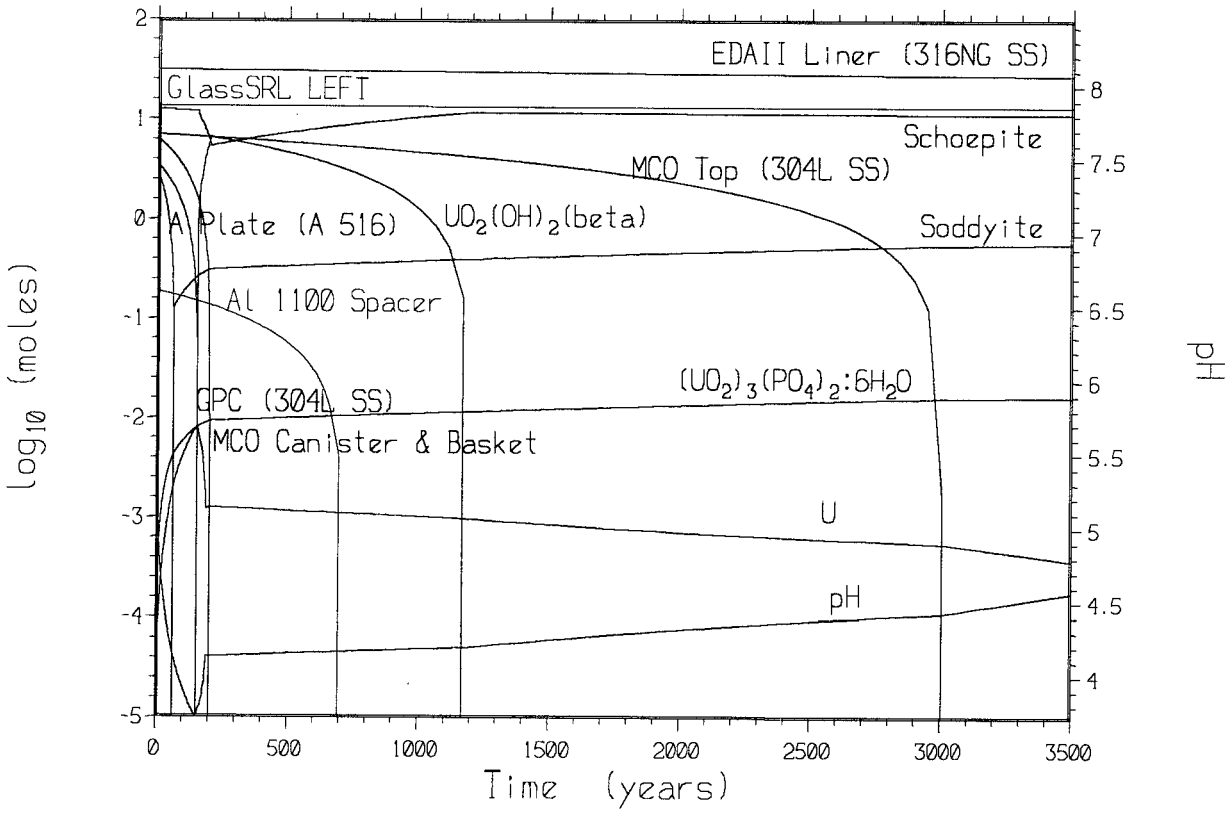

Figure 4. Predicted Concentration of Major Waste Package Components, Precipitated U Minerals, Total U in Solution, and pH as a Function of Time Early in Case 2 (n40h2111)

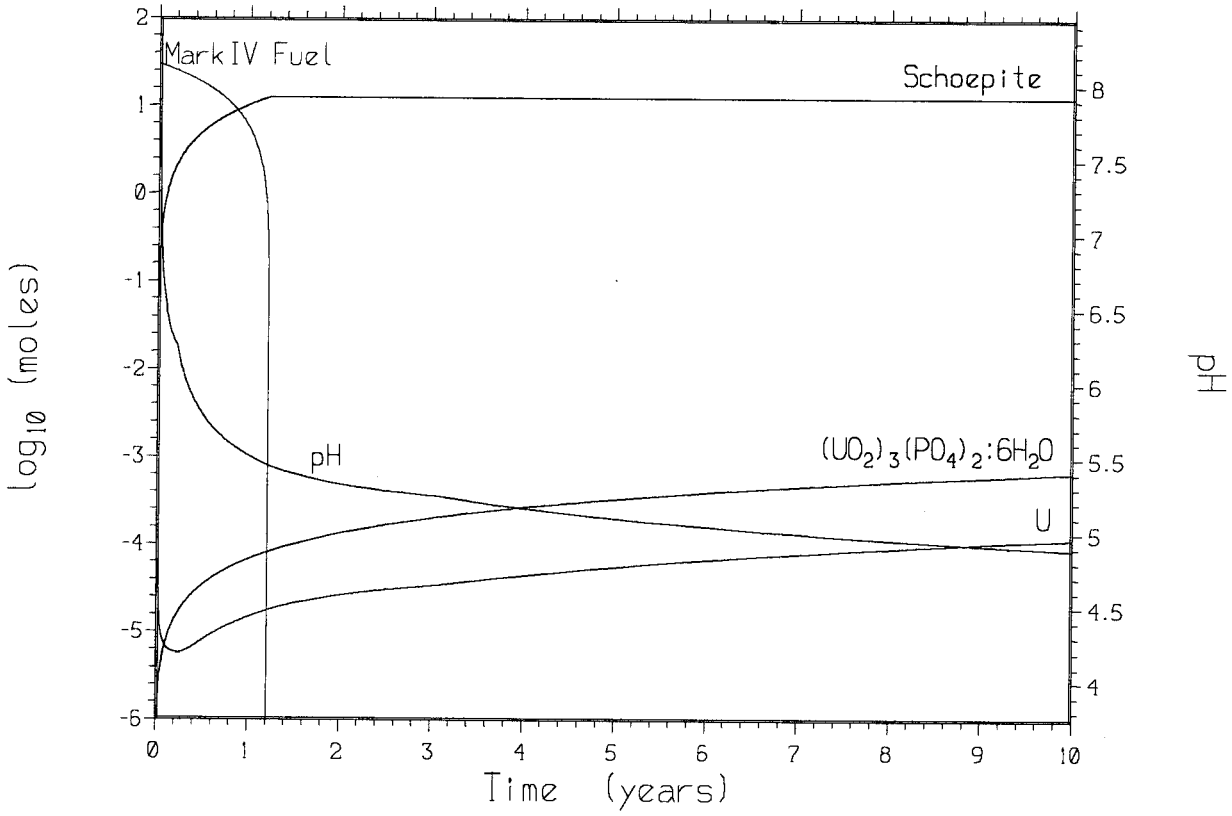

Figure 5. Predicted Concentration of N-Reactor SNF, Precipitated U Minerals, Total U in Solution, and pH as a Function of Time Early in Case 2 (n40h2111)

Table 13. Predicted Elemental Composition of Corrosion Products (kg), Total Mass (kg) and Density in Selected Years for Case 3 (n40h1112, n41h1112, n42h1112)

Years	318	51325	101090	633790
Element				
O	4.844E+03	6.410E+03	7.127E+03	1.216E+04
Al	3.679E-02	5.201E+00	1.002E+01	6.255E+01
B	2.997E-15	1.501E-17	0.000E+00	0.000E+00
Ba	2.154E-03	2.603E-01	5.101E-01	3.222E+00
Ca	2.639E-02	3.023E+00	6.998E+00	5.738E+01
Cr	0.000E+00	9.856E-02	1.931E-01	2.406E-17
Cu	8.393E+01	1.779E+02	1.757E+02	1.651E+02
Fe	1.223E+03	4.368E+03	5.708E+03	1.417E+04
H	2.159E+02	2.171E+02	2.182E+02	2.325E+02
C	1.189E-10	1.440E-10	1.811E-10	2.818E-01
P	4.419E-01	2.591E+00	3.544E+00	9.840E+00
Mg	5.704E-04	5.098E-01	1.239E+00	1.171E+01
Mn	1.337E+01	1.061E+02	1.457E+02	3.968E+02
Mo	0.000E+00	0.000E+00	3.823E+00	2.629E+01
Ni	0.000E+00	0.000E+00	2.906E+01	5.113E+02
S	6.381E-02	1.484E-17	0.000E+00	1.484E-17
Si	4.356E+00	1.080E+02	1.881E+02	9.878E+02
U	1.275E+04	1.275E+04	1.275E+04	1.278E+04
Total (kg)	1.913E+04	2.415E+04	2.637E+04	4.157E+04
Density (g/cm^3)	4.912	4.935	4.925	4.807

Table 14. Predicted Solution Elemental Composition (mole kg^{-1}) and pH in Selected Years for Case 3 (n40h1112, n41h1112, n42h1112)

Years	318	51325	101090	633790
pH	5.58	5.84	6.27	7.06
Element				
Al	8.193E-11	7.232E-12	1.830E-13	4.331E-15
B	6.857E-04	8.557E-04	8.200E-04	1.231E-03
Ba	2.315E-07	7.311E-07	6.285E-07	7.046E-07
Ca	2.718E-04	2.736E-04	2.193E-04	3.762E-05
Cl	2.014E-04	2.014E-04	2.014E-04	2.014E-04
Cr	1.513E-02	2.158E-02	5.383E-03	7.037E-04
Cu	6.115E-04	2.032E-04	2.167E-05	6.131E-07
F	1.187E-04	1.197E-04	1.195E-04	1.219E-04
Fe	8.077E-12	5.618E-12	2.617E-12	1.317E-12
C	3.512E-05	4.648E-05	6.662E-05	2.324E-04
P	1.758E-08	2.685E-08	5.037E-08	3.448E-07
K	3.028E-04	3.467E-04	3.375E-04	4.435E-04
Li	4.849E-06	6.915E-06	6.915E-06	6.915E-06
Mg	1.543E-04	1.518E-04	1.266E-04	2.200E-05
Mn	8.062E-11	2.805E-11	2.940E-12	6.802E-14
Mo	2.616E-04	3.731E-04	2.944E-04	1.347E-03
N	4.448E-04	5.741E-04	2.576E-04	1.554E-04
Na	3.331E-03	3.662E-03	3.592E-03	4.405E-03
Ni	7.581E-03	1.081E-02	2.199E-03	5.077E-05
S	1.575E-03	2.598E-04	2.178E-04	2.101E-04
Si	1.606E-04	1.857E-04	1.857E-04	1.863E-04
U	1.441E-05	8.418E-06	6.349E-06	1.529E-05

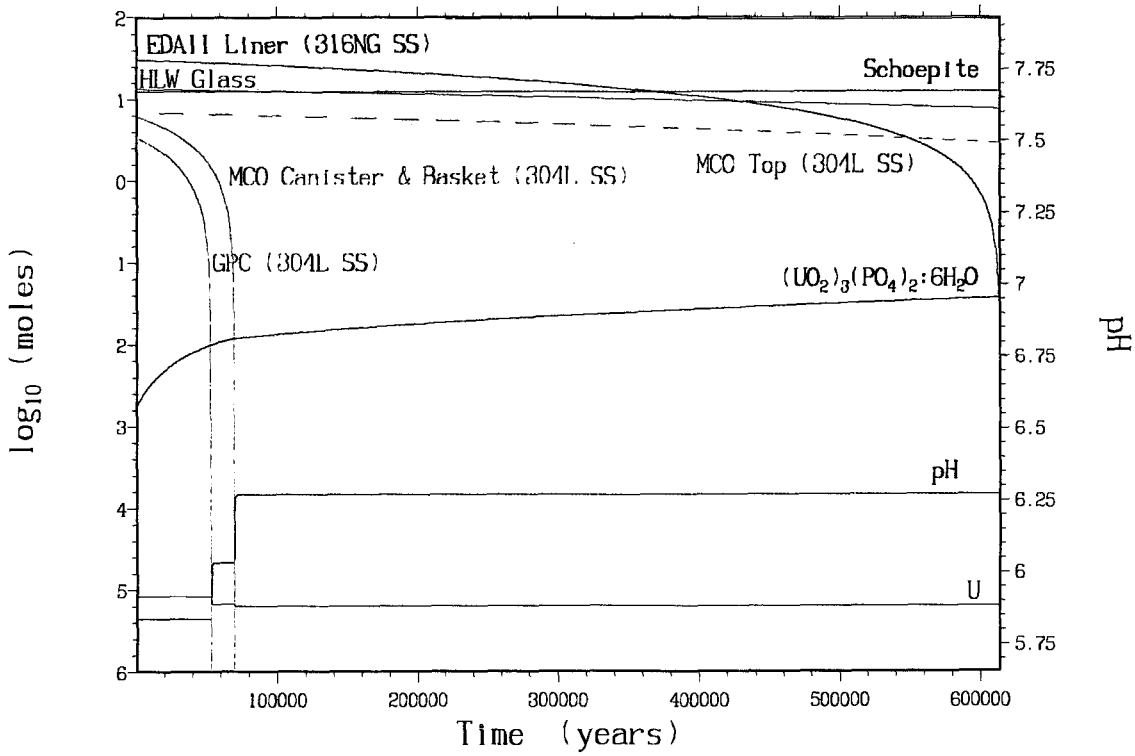

Figure 6. Predicted Concentration of Major Waste Package Components, Precipitated U Minerals, Total U in Solution, and pH as a Function of Time During Case 3 (n40h1112)

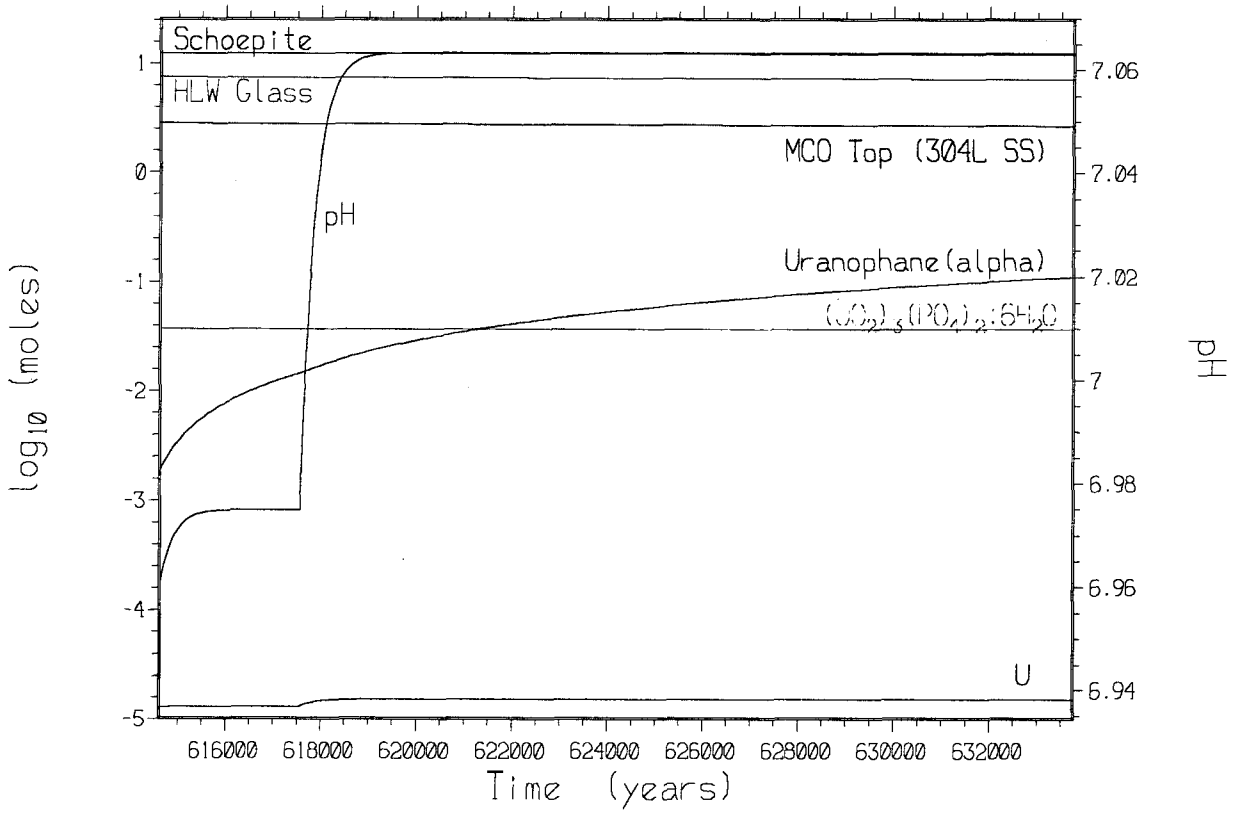

Figure 7. Predicted Concentration of Major Waste Package Components, Precipitated U Minerals, Total U in Solution, and pH as a Function of Time at the End of Case 3 (n42H1112)

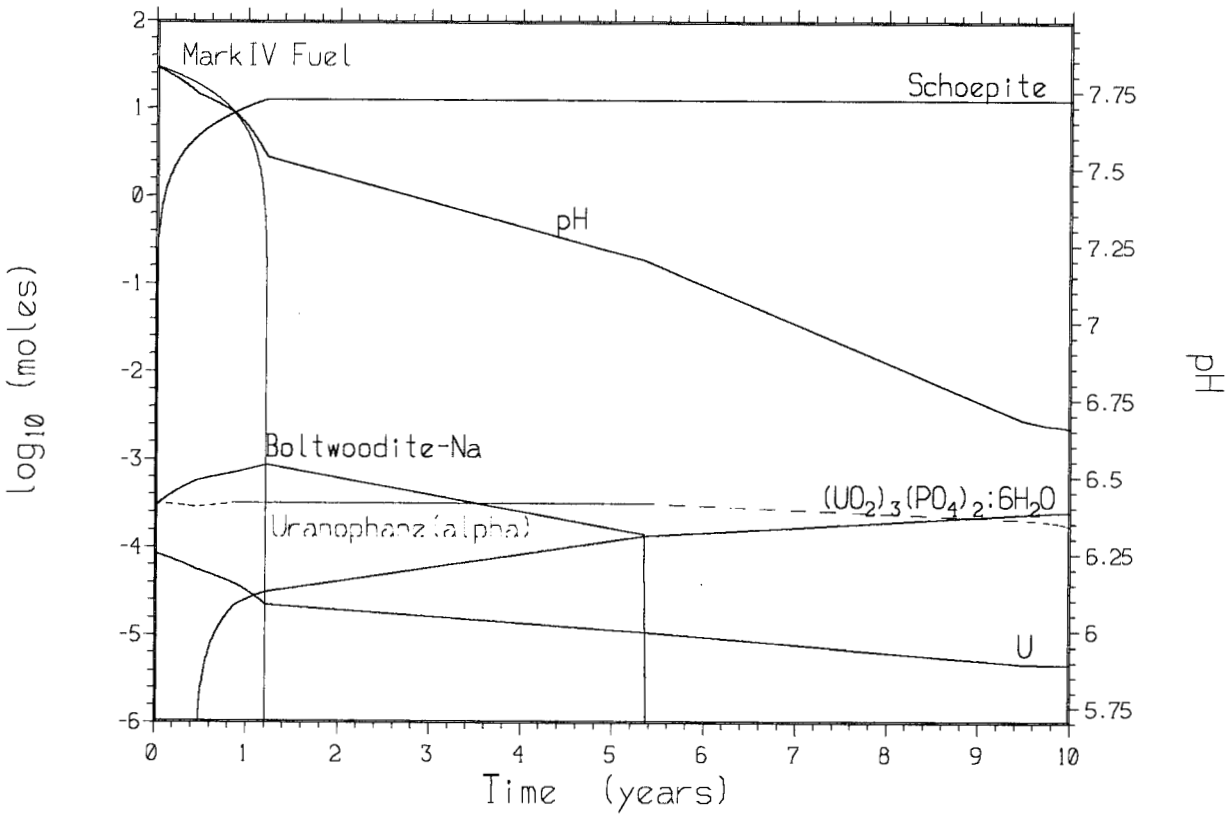

Figure 8. Predicted Concentration of N-Reactor SNF, Precipitated U Minerals, Total U in Solution, and pH as a Function of Time Early in Case 3 (n40h1112)

Table 15. Predicted Elemental Composition of Corrosion Products (kg), Total Mass (kg) and Density in Selected Years for Case 4 (n10h1111)

Years	1656	122610	634310
Element			
O	3.865E+03	6.604E+03	1.124E+04
Al	1.964E-01	1.337E+01	6.475E+01
B	2.522E-15	9.388E-13	0.000E+00
Ba	1.233E-02	8.471E-01	4.119E+00
Ca	9.560E-02	5.263E+00	2.752E+01
Cl	0.000E+00	0.000E+00	1.603E-13
Cr	0.000E+00	3.207E-01	1.559E+00
Cu	2.122E+02	2.036E+02	1.927E+02
F	0.000E+00	0.000E+00	3.861E-13
Fe	1.310E+03	6.801E+03	1.491E+04
H	1.628E+02	1.659E+02	1.782E+02
C	0.000E+00	0.000E+00	9.231E-12
P	5.001E-01	4.237E+00	1.002E+01
K	6.418E-03	3.749E+00	1.975E+01
Li	0.000E+00	0.000E+00	1.328E-15
Mg	6.780E-02	4.353E+00	2.144E+01
Mn	1.591E+01	1.778E+02	4.185E+02
Mo	1.551E-01	1.260E+01	6.225E+01
N	0.000E+00	0.000E+00	7.225E-14
Na	0.000E+00	9.591E-01	7.510E+00
Ni	0.000E+00	3.437E+01	4.017E+02
S	9.257E-02	0.000E+00	1.449E-11
Si	6.833E+00	2.017E+02	8.174E+02
U	9.609E+03	9.619E+03	9.658E+03
Total (kg)	1.518E+04	2.385E+04	3.804E+04
Density (g/cm^3)	4.936	4.947	4.855

Table 16. Predicted Solution Elemental Composition (mole kg^{-1}) and pH in Selected Years for Case 4 (n10h1111)

Years	1656	122610	634310
pH	5.53	5.87	6.68
Element			
Al	1.866E-10	1.177E-11	2.087E-14
B	4.502E-03	8.359E-03	9.421E-03
Ba	5.060E-07	5.961E-07	3.388E-07
Ca	1.555E-04	6.426E-05	9.161E-05
Cl	2.014E-04	2.014E-04	2.014E-04
Cr	1.015E-01	5.382E-02	7.020E-03
Cu	1.180E-03	2.338E-04	3.725E-06
F	1.410E-04	1.635E-04	1.697E-04
Fe	9.919E-12	5.720E-12	1.690E-12
C	3.175E-05	4.781E-05	1.199E-04
P	1.676E-08	2.906E-08	1.282E-07
K	1.250E-03	1.776E-03	1.173E-03
Li	3.131E-06	6.915E-06	6.915E-06
Mg	7.807E-05	1.265E-04	5.251E-05
Mn	1.606E-10	3.231E-11	4.852E-13
Mo	1.398E-03	3.007E-03	8.164E-04
N	2.173E-03	1.301E-03	2.795E-04
Na	1.088E-02	1.838E-02	1.236E-02
Ni	5.070E-02	2.423E-02	3.622E-04
S	2.186E-03	4.582E-04	3.389E-04
Si	1.511E-04	1.856E-04	1.859E-04
U	1.808E-05	9.097E-06	8.810E-06

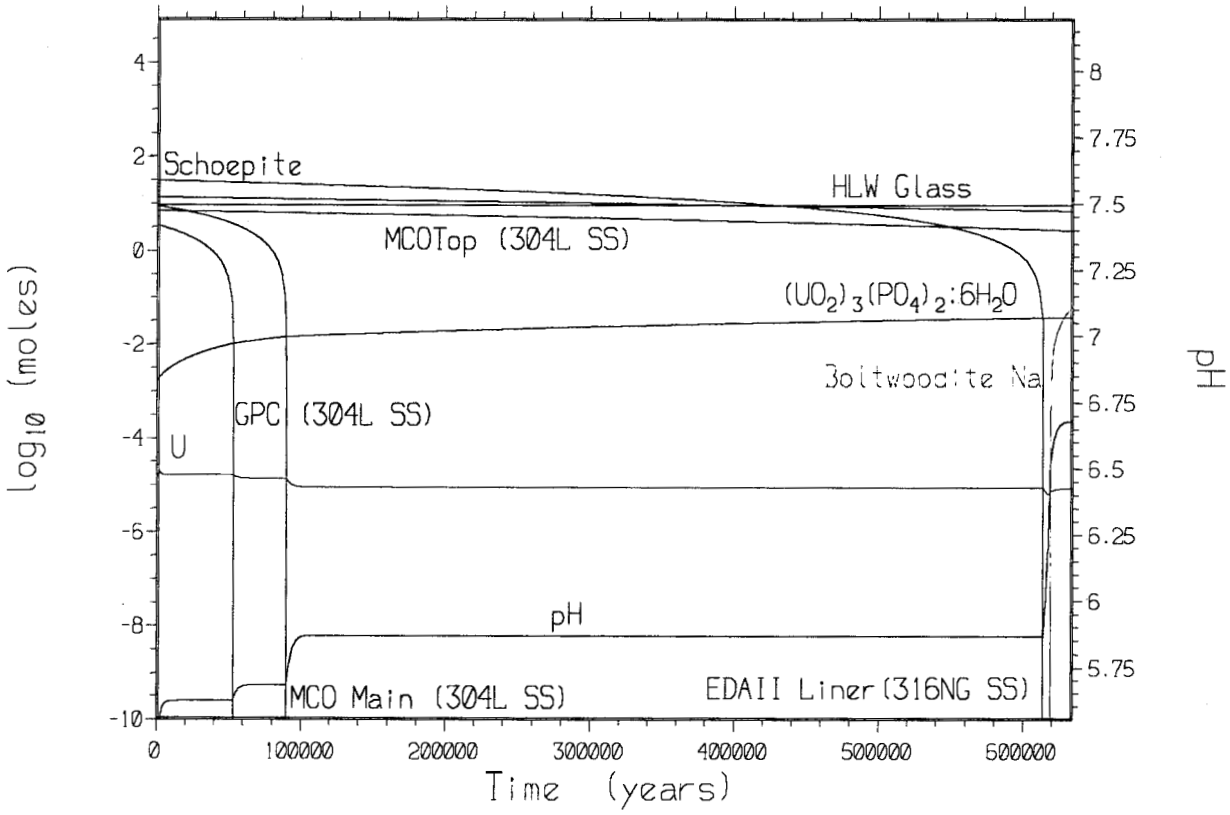

Figure 9. Predicted Concentration of Major Waste Package Components, Precipitated U Minerals, Total U in Solution, and pH as a Function of Time During Case 4 (n10H1111)

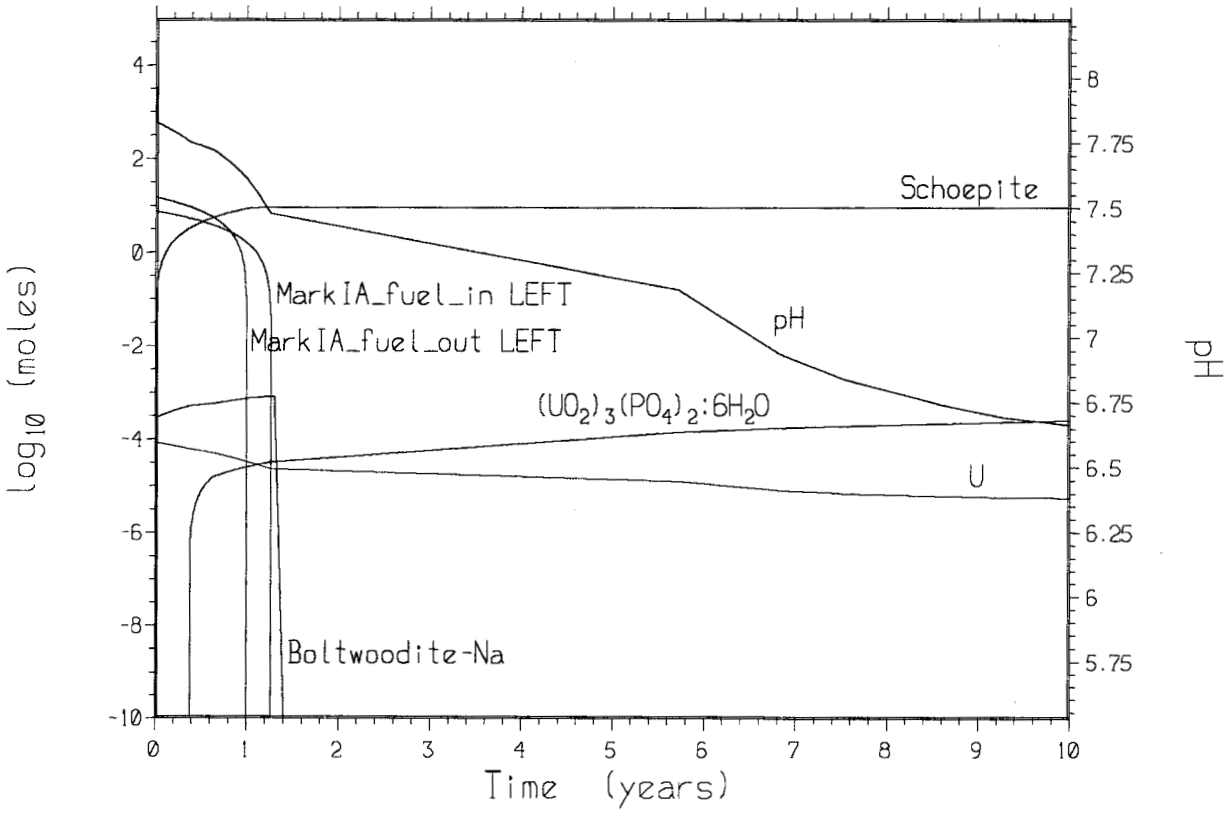

Figure 10. Predicted Concentration of N-Reactor SNF, Precipitated U Minerals, Total U in Solution, and pH as a Function of Time Early in Case 4 (n10H1111)

Table 17. Predicted Elemental Composition of Corrosion Products (kg), Total Mass (kg) and Density in Selected Years for Case 5 (n10h2111)

Years	155	49916	634320
Element			
O	4.960E+03	1.056E+04	1.274E+04
Al	9.041E-02	8.418E+00	1.342E+02
B	3.403E-16	7.083E-12	5.473E-19
Ba	5.044E-03	5.343E-01	8.696E+00
Ca	6.831E-02	3.241E+00	4.945E+01
Cr	2.981E-07	0.000E+00	0.000E+00
Cu	6.540E+00	1.523E+02	1.523E+02
F	0.000E+00	0.000E+00	2.182E+00
Fe	3.888E+03	1.546E+04	1.598E+04
H	1.580E+02	1.647E+02	1.862E+02
C	1.367E-12	0.000E+00	7.605E-01
P	2.206E+00	1.013E+01	1.067E+01
K	7.238E-17	2.708E+00	3.627E+01
Mg	1.125E-17	2.255E+00	4.128E+01
Mn	9.175E+01	4.415E+02	4.415E+02
Mo	1.635E-01	5.013E+00	0.000E+00
Na	1.702E-16	5.446E+00	7.218E+02
Ni	0.000E+00	9.762E+01	9.753E+01
S	1.101E+00	1.247E-01	1.113E-17
Si	3.430E+01	2.780E+02	1.480E+03
U	9.602E+03	9.614E+03	9.620E+03
Total (kg)	1.874E+04	3.681E+04	4.170E+04
Density (g/cm^3)	4.993	5.030	4.674

Table 18. Predicted Solution Elemental Composition (mole kg^{-1}) and pH in Selected Years for Case 5 (n10h2111)

Years	155	49916	634320
pH	3.81	7.03	8.21
Element			
Al	1.348E-06	5.592E-15	1.038E-07
B	2.612E-03	1.032E-02	1.239E-05
Ba	1.372E-06	3.531E-07	3.687E-09
Ca	7.761E-05	3.554E-05	5.610E-06
Cl	2.014E-04	2.014E-04	2.014E-04
Cr	3.285E+00	5.612E-04	1.000E-16
Cu	1.327E-01	7.546E-07	7.478E-08
F	1.299E-04	1.749E-04	1.147E-04
Fe	3.371E-10	1.340E-12	1.138E-12
C	3.318E-06	2.182E-04	3.752E-03
P	1.342E-08	3.145E-07	1.156E-06
K	8.002E-04	7.440E-04	2.522E-03
Li	3.667E-07	6.915E-06	6.915E-06
Mg	3.800E-04	2.091E-05	2.362E-04
Mn	1.135E-07	8.439E-14	5.594E-16
Mo	3.566E-03	1.569E-03	1.000E-16
N	6.444E-02	1.538E-04	1.416E-04
Na	7.141E-03	5.292E-03	1.829E-03
Ni	1.540E+00	6.199E-05	2.601E-07
S	3.764E-03	6.730E-04	1.915E-04
Si	9.532E-05	1.862E-04	3.689E-05
U	6.891E-03	1.446E-05	5.085E-04

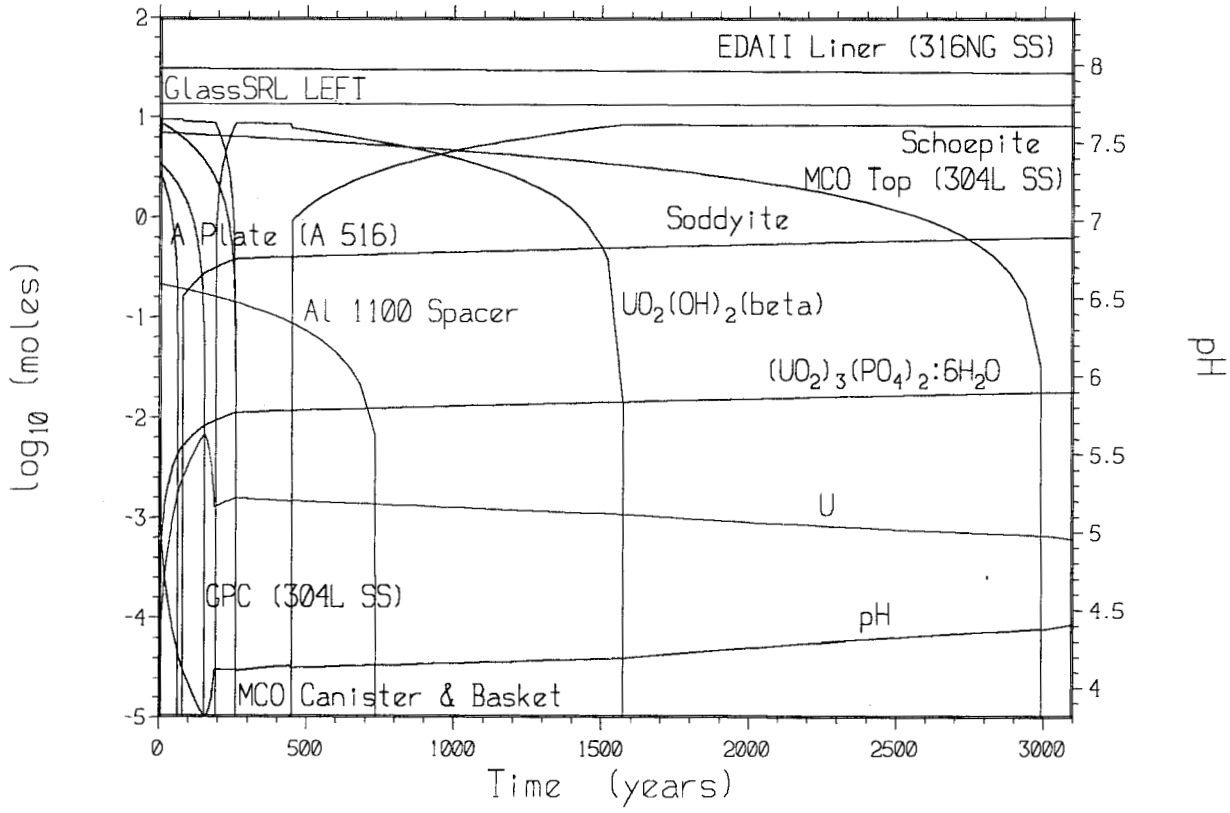

Figure 11. Predicted Concentration of Major Waste Package Components, Precipitated U Minerals, Total U in Solution, and pH as a Function of Time Early in Case 5 (n10H2111)

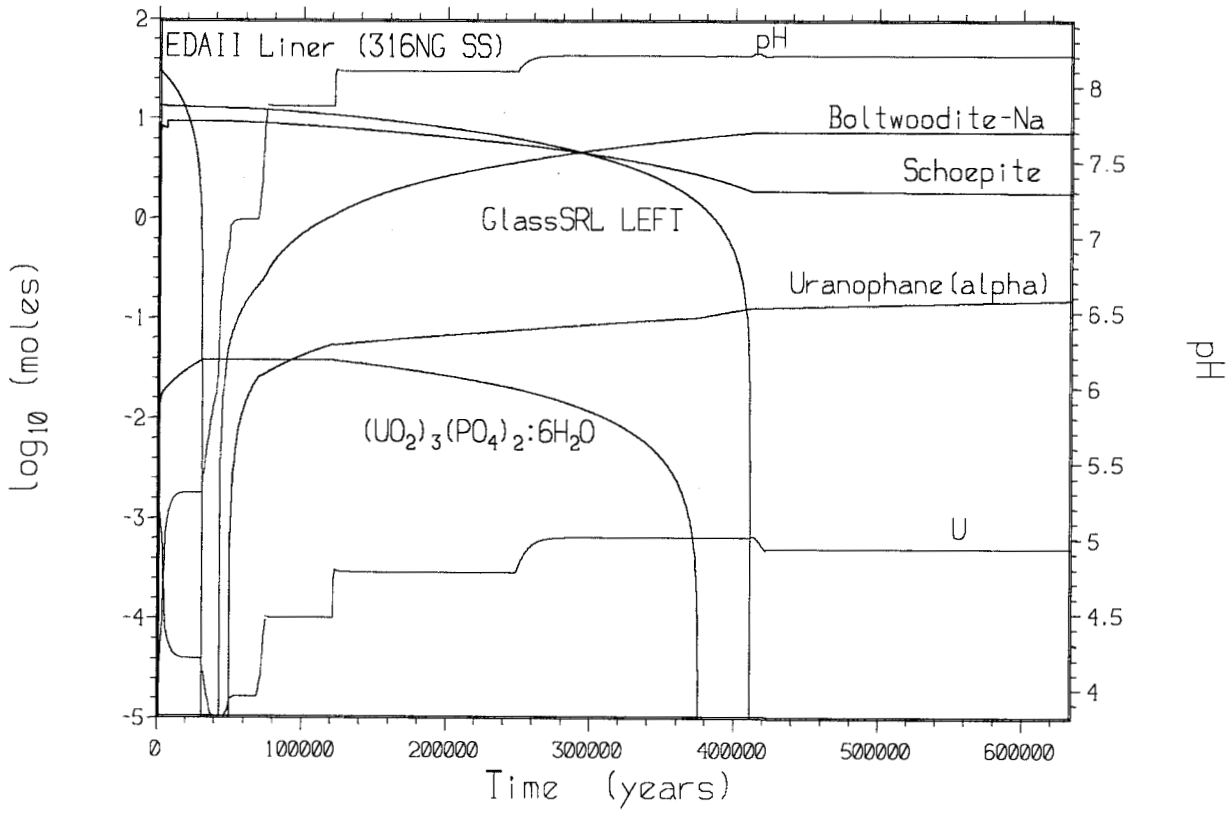

Figure 12. Predicted Concentration of Major Waste Package Components, Precipitated U Minerals, Total U in Solution, and pH as a Function of Time During Case 5 (n10H2111)

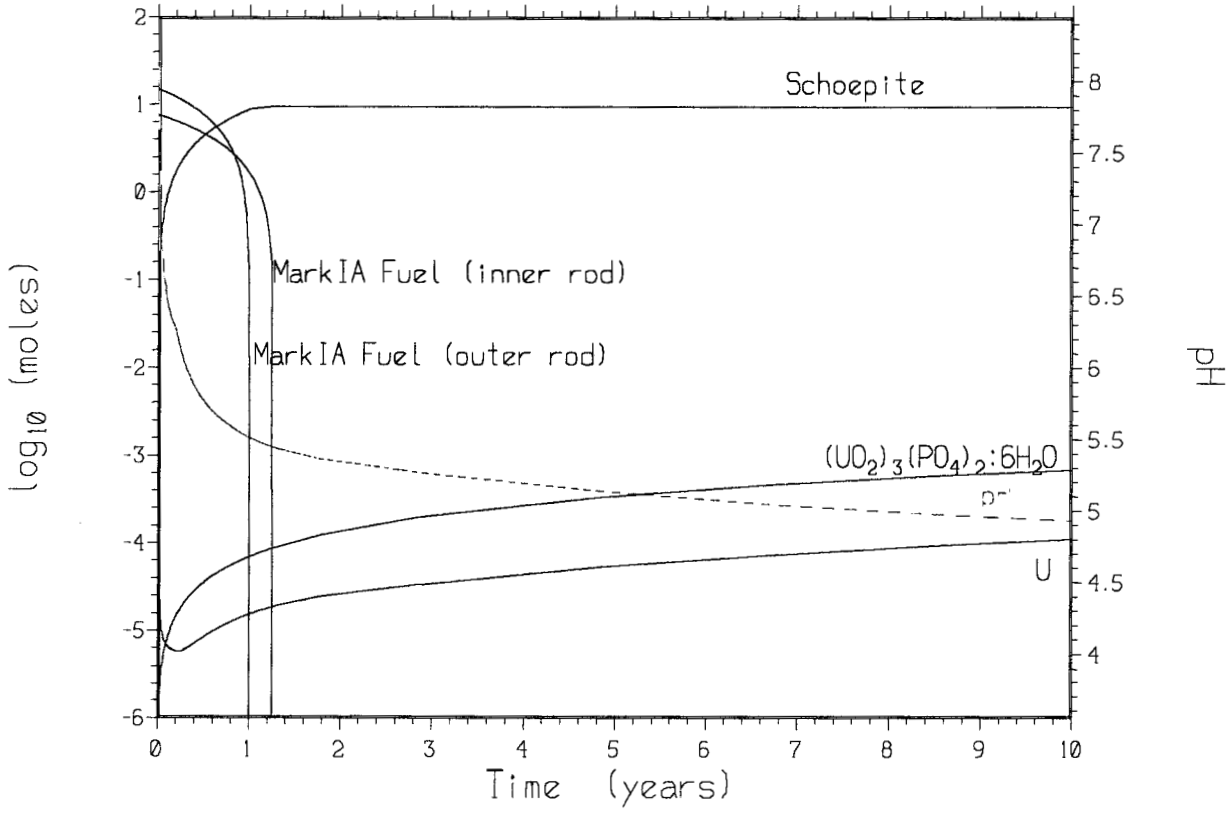

Figure 13. Predicted Concentration of N-Reactor SNF, Precipitated U Minerals, Total U in Solution, and pH as a Function of Time Early in Case 5 (n10H2111)

Table 19. Predicted Elemental Composition of Corrosion Products (kg), Total Mass (kg) and Density in Selected Years for Case 6 (n10h1112, n11h1112, n12h1112)

Years	317	102350	633820
Element			
O	3.791E+03	6.423E+03	1.145E+04
Al	3.686E-02	1.019E+01	6.259E+01
B	3.357E-15	0.000E+00	0.000E+00
Ba	2.137E-03	5.179E-01	3.224E+00
Ca	2.638E-02	6.519E+00	5.679E+01
Cr	0.000E+00	1.961E-01	2.406E-17
Cu	8.872E+01	1.978E+02	1.872E+02
Fe	1.224E+03	6.464E+03	1.490E+04
H	1.628E+02	1.651E+02	1.794E+02
C	0.000E+00	0.000E+00	2.820E-01
P	4.423E-01	4.046E+00	1.033E+01
Mg	6.011E-04	1.101E+00	1.155E+01
Mn	1.338E+01	1.679E+02	4.185E+02
Mo	0.000E+00	1.839E+00	2.411E+01
Ni	0.000E+00	1.161E+01	4.926E+02
S	6.007E-02	0.000E+00	1.113E-17
Si	4.361E+00	1.985E+02	9.963E+02
U	9.609E+03	9.614E+03	9.643E+03
Total (kg)	1.489E+04	2.327E+04	3.843E+04
Density (g/cm^3)	4.923	4.946	4.811

Table 20. Predicted Solution Elemental Composition (mole kg^{-1}) and pH in Selected Years for Case 6 (n10h1112, n11h1112, n12h1112)

Years	317	102350	633820
pH	5.57	6.27	7.06
Element			
Al	8.373E-11	1.830E-13	4.331E-15
B	6.882E-04	8.200E-04	1.231E-03
Ba	2.474E-07	6.285E-07	7.046E-07
Ca	2.718E-04	2.193E-04	3.762E-05
Cl	2.014E-04	2.014E-04	2.014E-04
Cr	1.567E-02	5.383E-03	7.037E-04
Cu	6.518E-04	2.167E-05	6.131E-07
F	1.187E-04	1.195E-04	1.219E-04
Fe	8.496E-12	2.617E-12	1.317E-12
C	3.634E-05	6.662E-05	2.324E-04
P	1.814E-08	5.037E-08	3.448E-07
K	3.034E-04	3.375E-04	4.435E-04
Li	4.835E-06	6.915E-06	6.915E-06
Mg	1.542E-04	1.266E-04	2.200E-05
Mn	8.606E-11	2.940E-12	6.802E-14
Mo	2.609E-04	2.944E-04	1.347E-03
N	4.554E-04	2.576E-04	1.554E-04
Na	3.335E-03	3.592E-03	4.405E-03
Ni	7.832E-03	2.199E-03	5.077E-05
S	1.581E-03	2.178E-04	2.101E-04
Si	1.666E-04	1.857E-04	1.863E-04
U	1.491E-05	6.349E-06	1.529E-05

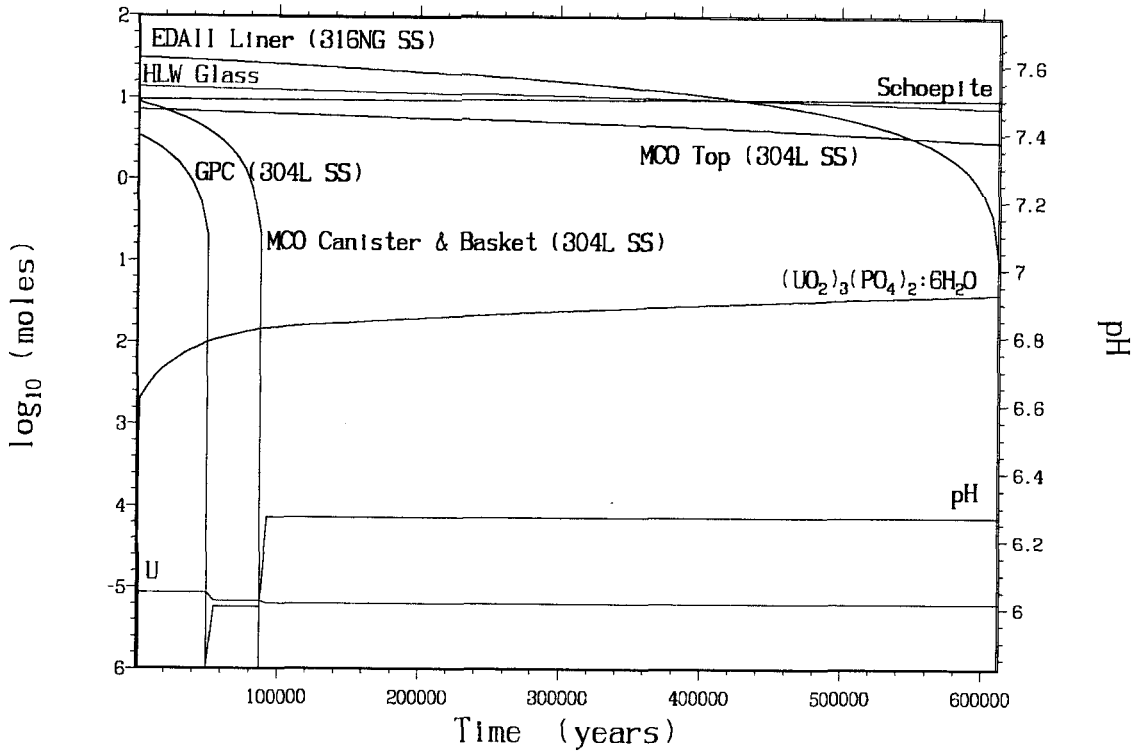

Figure 14. Predicted Concentration of Major Waste Package Components, Precipitated U Minerals, Total U in Solution, and pH as a Function of Time During Case 6 (n10H1112)

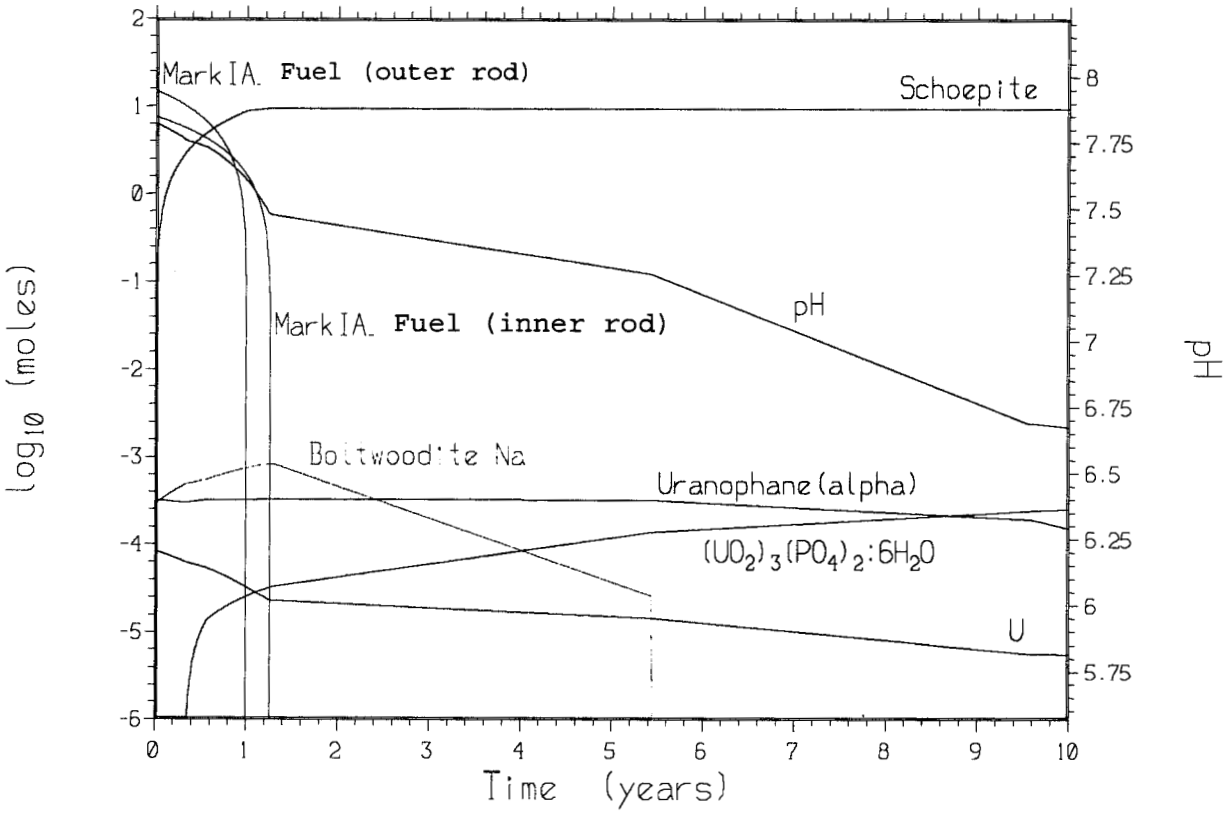

Figure 15. Predicted Concentration of N-Reactor SNF, Precipitated U Minerals, Total U in Solution, and pH as a Function of Time Early in Case 6 (n10H1112)

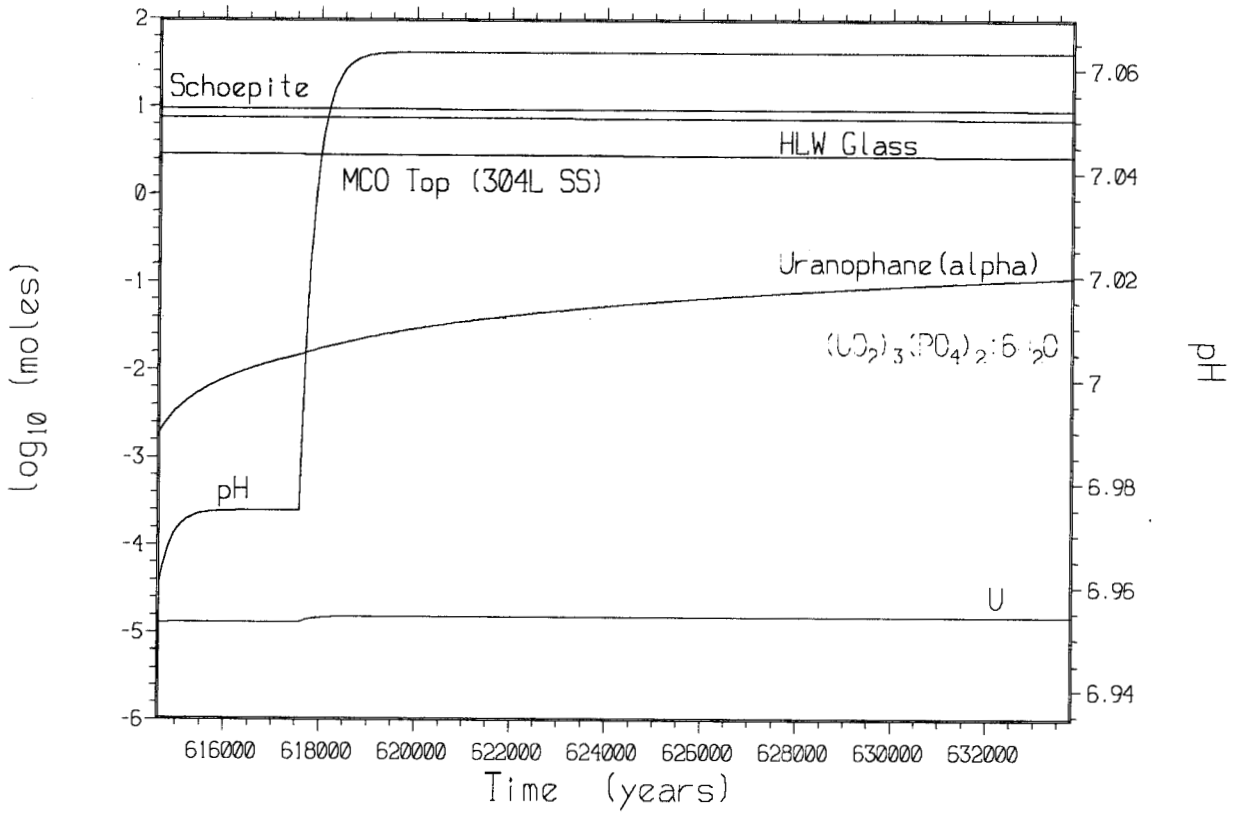

Figure 16. Predicted Concentration of Major Waste Package Components, Precipitated U Minerals, Total U in Solution, and pH as a Function of Time at the End of Case 6 (n12H1112)

Table 21. Predicted Elemental Composition of Corrosion Products (kg), Total Mass (kg) and Density in Selected Years for Case 7 (n10#1111)

Years	1656	301830	633810
Element			
O	3.865E+03	8.274E+03	1.124E+04
Al	1.963E-01	3.131E+01	6.470E+01
B	2.522E-15	0.000E+00	0.000E+00
Ba	1.233E-02	1.989E+00	4.115E+00
Ca	9.560E-02	1.307E+01	2.750E+01
Cl	0.000E+00	0.000E+00	1.953E-13
Cr	0.000E+00	7.531E-01	1.558E+00
Cu	2.122E+02	1.996E+02	1.927E+02
F	0.000E+00	2.198E-18	4.707E-13
Fe	1.310E+03	9.741E+03	1.491E+04
H	1.628E+02	1.702E+02	1.782E+02
C	2.758E-12	5.776E-12	6.424E-12
P	5.001E-01	6.332E+00	1.002E+01
K	6.461E-03	9.094E+00	1.971E+01
Li	0.000E+00	0.000E+00	1.618E-15
Mg	6.778E-02	1.030E+01	2.142E+01
Mn	1.591E+01	2.652E+02	4.185E+02
Mo	1.553E-01	3.128E+01	6.231E+01
N	0.000E+00	3.888E-17	8.810E-14
Na	0.000E+00	1.848E+00	7.366E+00
Ni	0.000E+00	1.658E+02	4.016E+02
S	9.282E-02	0.000E+00	1.766E-11
Si	6.832E+00	4.184E+02	8.169E+02
U	9.609E+03	9.633E+03	9.658E+03
Total (kg)	1.518E+04	2.897E+04	3.803E+04
Density (g/cm^3)	4.936	4.905	4.855

Table 22. Predicted Solution Elemental Composition (mole kg^{-1}) and pH in Selected Years for Case 7 (n10#1111)

Years	1656	301830	633810
pH	5.53	5.87	6.68
Element			
Al	1.867E-10	1.177E-11	2.088E-14
B	4.501E-03	8.359E-03	9.417E-03
Ba	5.060E-07	5.961E-07	3.387E-07
Ca	1.555E-04	6.426E-05	9.167E-05
Cl	2.014E-04	2.014E-04	2.014E-04
Cr	1.015E-01	5.382E-02	7.023E-03
Cu	1.180E-03	2.338E-04	3.728E-06
F	1.410E-04	1.635E-04	1.697E-04
Fe	9.917E-12	5.720E-12	1.691E-12
C	3.173E-05	4.781E-05	1.199E-04
P	1.675E-08	2.906E-08	1.282E-07
K	1.249E-03	1.776E-03	1.173E-03
Li	3.131E-06	6.915E-06	6.915E-06
Mg	7.804E-05	1.265E-04	5.255E-05
Mn	1.605E-10	3.231E-11	4.855E-13
Mo	1.398E-03	3.007E-03	8.160E-04
N	2.173E-03	1.301E-03	2.796E-04
Na	1.088E-02	1.838E-02	1.236E-02
Ni	5.070E-02	2.423E-02	3.625E-04
S	2.185E-03	4.582E-04	3.388E-04
Si	1.510E-04	1.856E-04	1.859E-04
U	1.808E-05	9.097E-06	8.808E-06

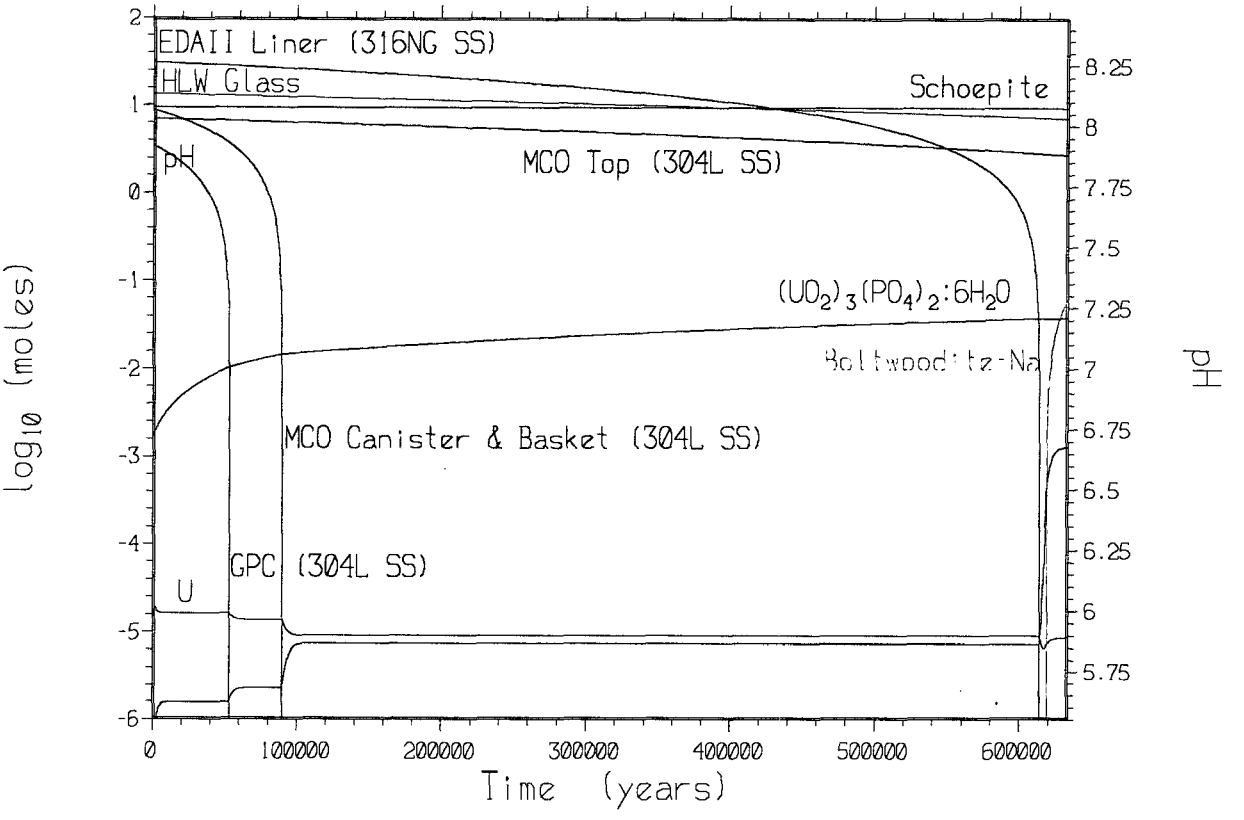

Figure 17. Predicted Concentration of Major Waste Package Components, Precipitated U Minerals, Total U in Solution, and pH as a Function of Time During Case 7 (n10#1111)

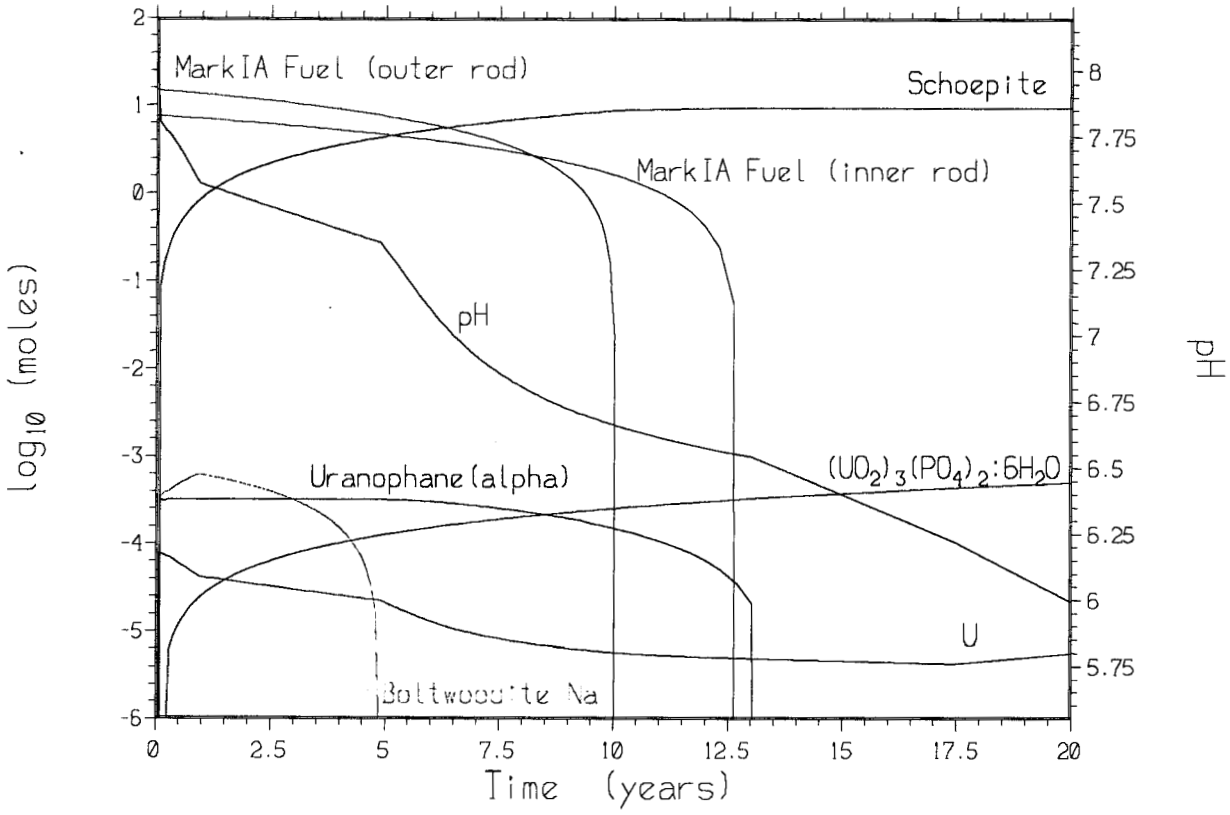

Figure 18. Predicted Concentration of N-Reactor SNF, Precipitated U Minerals, Total U in Solution, and pH as a Function of Time Early in Case 7 (n10#1111)

Table 23. Predicted Elemental Composition of Corrosion Products (kg), Total Mass (kg) and Density in Selected Years for Case 8 (n10&1111, n11&1111)

Years	2014	105440	634090
Element			
O	6.460E+02	3.219E+03	8.023E+03
Al	2.430E-01	1.188E+01	6.614E+01
B	0.000E+00	0.000E+00	1.880E-13
Ba	1.521E-02	7.507E-01	4.208E+00
Ca	1.021E-01	4.564E+00	2.796E+01
Cl	3.365E-13	1.912E-13	0.000E+00
Cr	1.157E-07	2.842E-01	0.000E+00
Cu	2.121E+02	2.024E+02	1.910E+02
F	7.146E-12	3.961E-12	1.129E-01
Fe	1.333E+03	6.520E+03	1.492E+04
H	5.829E-02	2.848E+00	1.590E+01
C	1.676E-12	7.680E-12	3.680E-01
P	5.110E-01	3.937E+00	6.797E+00
K	4.832E-12	3.303E+00	1.976E+01
Li	1.548E-15	5.915E-16	0.000E+00
Mg	8.066E-02	3.838E+00	2.165E+01
Mn	1.658E+01	1.694E+02	4.185E+02
Mo	1.306E-01	1.092E+01	5.440E+01
N	1.995E-11	4.812E-12	0.000E+00
Na	1.544E-11	9.183E-01	4.766E+00
Ni	1.039E-10	2.794E+01	4.076E+02
S	3.551E-03	1.111E-11	0.000E+00
Si	7.547E+00	1.830E+02	8.304E+02
U	1.933E-01	9.461E+00	5.268E+01
Total (kg)	2.216E+03	1.038E+04	2.506E+04
Density (g/cm^3)	5.349	5.063	4.845

Table 24. Predicted Solution Elemental Composition (mole kg^{-1}) and pH in Selected Years for Case 8 (n10&1111, n11&1111)

Years	2014	105440	634090
pH	5.52	5.87	7.88
Element			
Al	2.020E-10	1.246E-11	1.020E-15
B	5.305E-03	8.375E-03	1.958E-02
Ba	6.354E-07	5.969E-07	2.626E-08
Ca	1.847E-04	6.447E-05	2.323E-05
Cl	2.014E-04	2.014E-04	2.014E-04
Cr	1.178E-01	5.408E-02	7.294E-03
Cu	1.474E-03	2.358E-04	1.764E-07
F	1.459E-04	1.636E-04	1.096E-14
Fe	1.251E-11	5.777E-12	1.139E-12
C	3.857E-05	4.714E-05	1.477E-03
P	2.042E-05	2.475E-05	2.606E-03
K	1.496E-03	1.779E-03	3.083E-03
Li	3.633E-06	6.915E-06	6.915E-06
Mg	9.312E-05	1.270E-04	5.239E-04
Mn	2.005E-10	3.248E-11	2.522E-15
Mo	1.715E-03	3.006E-03	6.636E-03
N	2.499E-03	1.306E-03	2.796E-04
Na	1.247E-02	1.841E-02	3.241E-02
Ni	5.882E-02	2.436E-02	1.801E-06
S	2.521E-03	4.590E-04	4.783E-04
Si	1.855E-04	1.855E-04	1.961E-04
U	3.147E-07	2.762E-07	6.337E-06

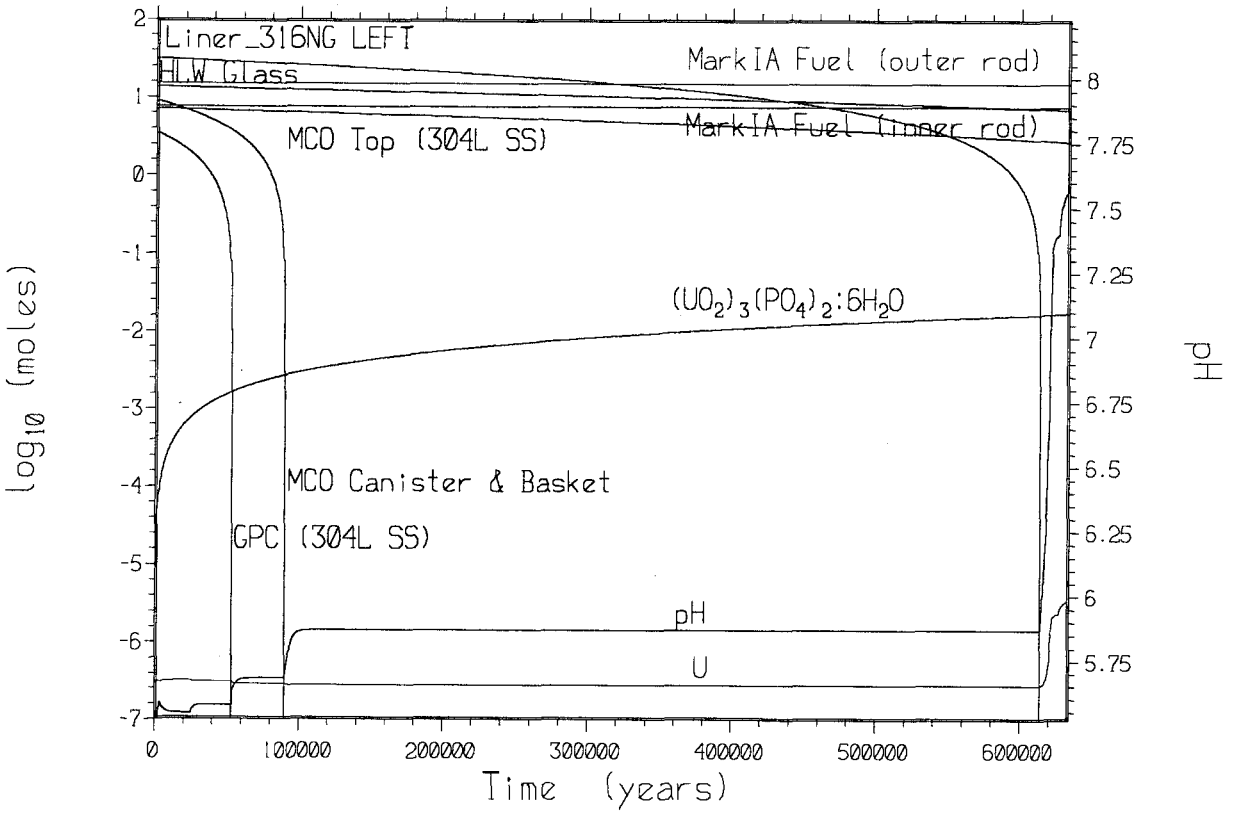

Figure 19. Predicted Concentration of Major Waste Package Components, Precipitated U Minerals, Total U in Solution, and pH as a Function of Time During Case 8 (n10&1111)

Case 9 predicted the corrosion of Mark IA SNF (assuming a decayed, instead of fresh, fuel composition in the WP) with low steel and high HLW glass degradation rates and low drip rates. Figure 20 shows the predicted concentration of major WP components, precipitated Np, Pu, and U Minerals, total Np, Pu, and U in solution, and pH as a function of time during Case 9 (n10h1211). The predicted soluble U concentration is fairly constant and is controlled mainly by the formation of schoepite ($UO_3:2H_2O$) with smaller amounts of $(UO_2)_3(PO_4)_2:6H_2O$ also precipitating. Sodium boltwoodite ($NaUO_2SiO_3OH:1.5H_2O$) is an important sink for U during the period from ~90,000 to 200,000 years, during and following the predicted complete dissolution of the HLW glass. Soluble Pu from SNF degradation is held to low levels by formation of PuO_2. The predicted soluble Np concentrations are similar to those of U from ~200,000 to 600,000 years. However, only a small amount of NpO_2 is predicted to form at the beginning of this period and the predicted amount of NpO_2 decreases through 6.35 x 10^5 years leading to large predicted losses of Np from the WP (Table 8). There is more than a five-fold decrease in the predicted kg of Np in the WP corrosion products between ~1.35 x 10^5 and ~6.35 x 10^5 years (shown in Table 25).

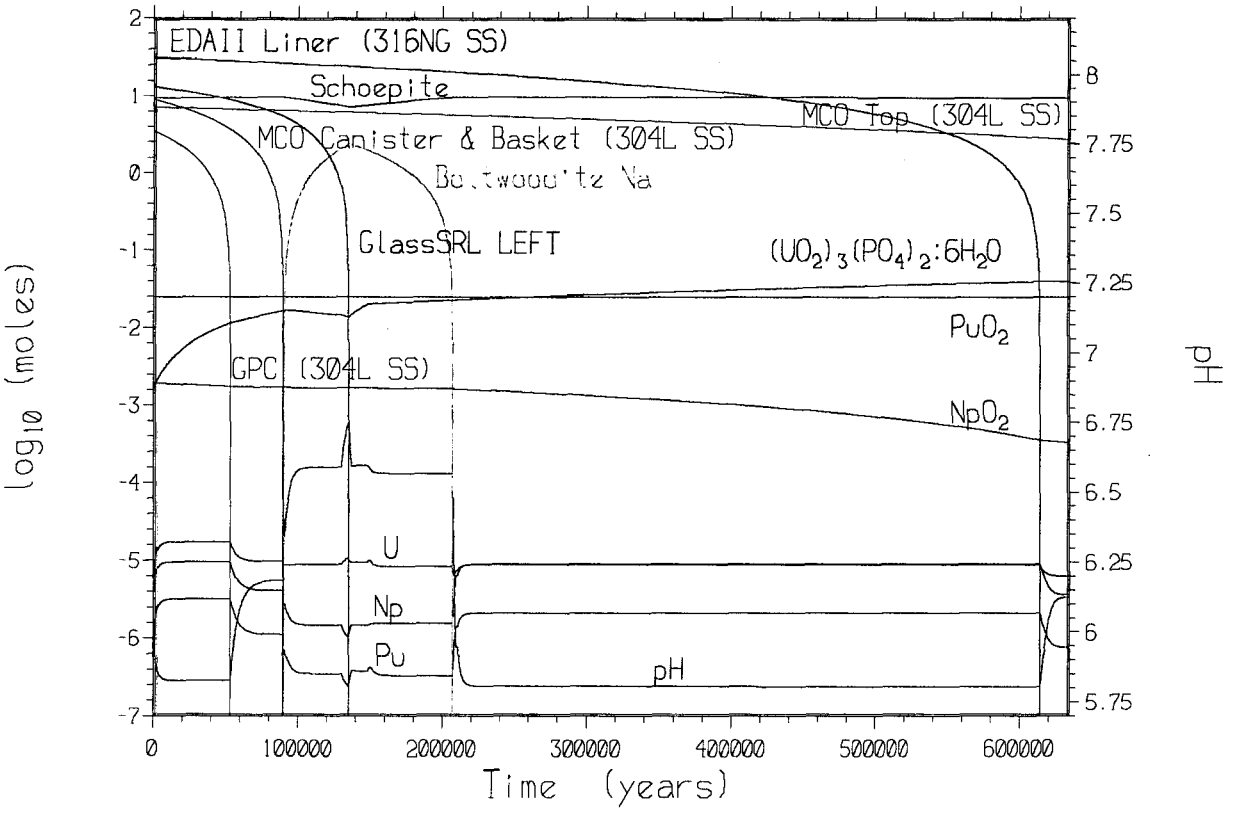

Figure 20. Predicted Concentration of Major Waste Package Components, Precipitated Np, Pu, and U Minerals, Total Np, Pu, and U in Solution, and pH as a Function of Time During Case 9 (n10h1211)

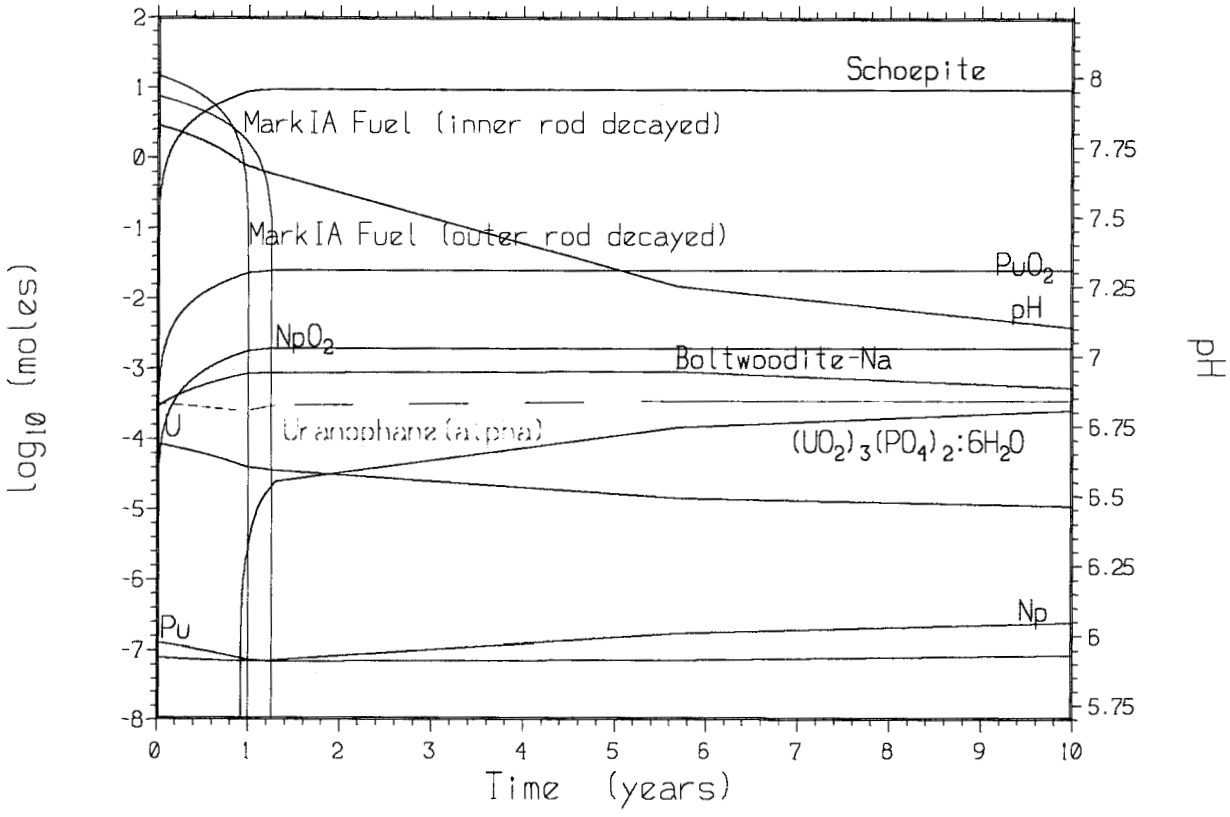

Figure 21. Predicted Concentration of N Reactor SNF, Precipitated Np, Pu, and U Minerals, Total Np, Pu, and U in Solution, and pH as a Function of Time Early in Case 9 (n10h1211)

Table 25. Predicted Elemental Composition of Corrosion Products (kg), Total Mass (kg) and Density in Selected Years for Case 9 (n10h1211)

Years	51305	134790	634080
Element			
O	6.107E+03	8.821E+03	1.238E+04
Al	4.529E+01	1.342E+02	1.341E+02
B	0.000E+00	3.845E-12	0.000E+00
Ba	2.937E+00	8.700E+00	8.635E+00
Ca	1.029E+01	3.120E+01	3.960E+01
Cl	2.317E-14	0.000E+00	1.635E-13
Cr	1.112E+00	3.294E+00	3.269E+00
Cu	2.107E+02	2.103E+02	1.977E+02
F	2.087E-12	3.239E-01	7.244E-12
Fe	4.652E+03	7.495E+03	1.520E+04
H	1.718E+02	1.887E+02	1.925E+02
C	0.000E+00	0.000E+00	7.690E-12
P	2.910E+00	5.175E+00	1.048E+01
K	1.676E+01	7.618E+01	3.901E+01
Li	4.131E-17	0.000E+00	2.116E-15
Mg	2.479E+00	1.737E+01	1.378E+01
Mn	1.095E+02	1.838E+02	4.185E+02
Mo	2.462E+01	6.650E+01	9.903E-14
N	6.692E-13	0.000E+00	1.470E-12
Na	2.003E+01	2.316E+02	1.143E+01
Ni	3.133E+02	6.845E+02	8.590E+02
Np	1.776E+00	1.692E+00	3.320E-01
Pu	2.543E+01	2.541E+01	2.509E+01
S	7.051E-12	0.000E+00	4.221E-12
Si	4.697E+02	1.338E+03	1.472E+03
U	9.569E+03	9.640E+03	9.638E+03
Total (kg)	2.176E+04	2.916E+04	4.065E+04
Density (g/cm^3)	4.764	4.526	4.708

Table 26. Predicted Solution Elemental Composition (mole kg^{-1}) and pH in Selected Years for Case 9 (n10h1211)

Years	51305	134790	634080
pH	5.83	6.75	6.12
Element			
Al	3.816E-05	4.060E-08	2.740E-07
B	7.363E-02	1.062E-01	1.239E-05
Ba	5.474E-07	1.434E-07	6.760E-07
Ca	1.078E-03	5.976E-04	5.997E-07
Cl	2.014E-04	2.014E-04	2.014E-04
Cr	2.239E-01	5.345E-02	7.056E-03
Cu	4.102E-04	4.535E-06	4.381E-05
F	5.445E-04	2.816E-04	1.148E-04
Fe	6.836E-12	1.685E-12	3.261E-12
C	4.691E-05	1.556E-04	5.738E-05
P	3.006E-08	2.678E-07	3.897E-08
K	1.357E-02	1.564E-02	9.573E-05
Li	6.915E-06	6.915E-06	6.915E-06
Mg	7.310E-03	1.015E-02	3.444E-07
Mn	5.658E-11	5.934E-13	5.987E-12
Mo	3.897E-04	3.632E-04	1.478E-06
N	4.629E-03	1.301E-03	2.795E-04
Na	1.364E-01	5.563E-02	1.010E-03
Ni	4.239E-02	4.416E-04	4.481E-03
Np	9.480E-06	1.026E-06	3.627E-06
Pu	3.186E-06	2.434E-07	7.638E-07
S	1.791E-03	1.802E-03	2.096E-04
Si	5.109E-05	4.133E-05	7.486E-05
U	1.732E-05	1.061E-05	6.320E-06

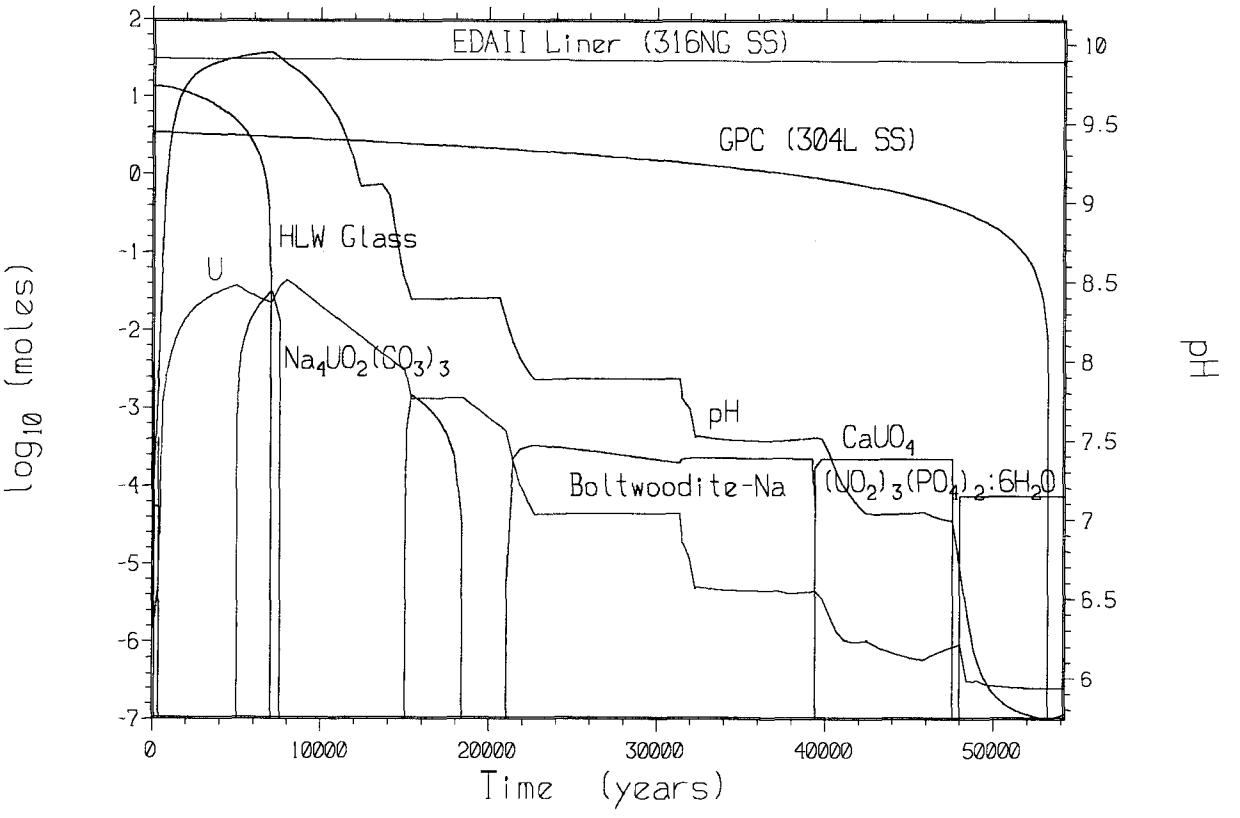

Figure 22. Predicted Concentration of Major Waste Package Components, Precipitated U Minerals, Total U in Solution, and pH as a Function of Time During the First-Stage of Case 10 (n10a1201)

Table 27. Predicted Mass Remaining of N-Reactor (U-metal) SNF WP Components in Selected Years for the First-stage of Case 10 (n10a1201)

Years	0	65	6953	54250
WP Component	**Mass (kg)**	**Mass (kg)**	**Mass (kg)**	**Mass (kg)**
HLW Glass	5766	5757	0	0
A-plate and MCO Stand (A516))	1224	0	0	0
EDAII Liner (316L SS)	13189	13188	13040	12024
GPC (304L SS))	1483	1481	1290	0

Source: "Nreactor_U.xls" sheet "Reactant Losses" (Attachment III)

Figure 22 shows the predicted partitioning of U between the WP solution and solid U-bearing phases during the degradation of HLW glass in the first stage of Case 10. The HLW glass degradation is complete before ~7000 years (Table 27) causing the WP solution to approach a

pH of 10 (Table 29). The predicted concentration of U in the WP solution remains high (10^{-3} to 10^{-1} molal) during the period of highest pH (~100 to 15,000 years). During the same time period, only small amounts of U-bearing solids are predicted to form (Figure 22 and Table 28) causing a predicted loss from the WP of most of the U from HLW glass degradation.

Degradation of stainless steel from the GPCs and the EDA II liner causes a predicted decrease in pH throughout the rest of the first stage (Figure 22, Table 27 and Table 29). The U in solution also decreases due to the formation of several U-bearing minerals.

Table 28. Predicted Elemental Composition of Corrosion Products (kg), Total Mass (kg) and Density in Selected Years for First Stage of Case 10 (n10a1201)

Years	65	6953	54251
Element			
O	5.332E+02	3.800E+03	3.474E+03
Al	2.045E-01	1.343E+02	1.343E+02
B	0.000E+00	1.541E+02	3.959E-13
Ba	1.320E-02	8.710E+00	8.708E+00
Ca	1.135E-01	3.762E+01	1.462E+01
Cl	1.102E-14	1.231E-17	0.000E+00
Cr	3.312E-11	0.000E+00	3.297E+00
F	1.076E-02	2.784E-01	4.522E-01
Fe	1.206E+03	1.987E+03	3.528E+03
H	4.902E-02	9.840E+01	2.722E+01
C	0.000E+00	3.253E+01	0.000E+00
P	1.857E-01	1.362E+00	2.307E+00
K	6.025E-02	9.912E+01	4.549E+01
Mg	7.047E-02	4.670E+01	3.269E+01
Mn	1.285E+01	1.964E+01	6.575E+01
Mo	1.593E-14	5.328E-16	1.282E+01
Na	5.516E-03	2.328E+02	0.000E+00
Ni	3.385E-01	3.726E+01	2.591E+02
S	3.083E-03	0.000E+00	0.000E+00
Si	5.592E+00	1.263E+03	1.285E+03
U	1.613E-01	3.324E+01	2.165E-01
Total (kg)	1.759E+03	7.985E+03	8.893E+03
Density (g/cm^3)	5.232	2.950	3.797

Table 29 shows that only ~0.2 kg of U is predicted to remain in the WP corrosion products by the end of the first stage of Case 10.

Table 29. Predicted Solution Elemental Composition (mole kg^{-1}) and pH in Selected Years for the First-stage of Case 10 (n10a1201)

Years	65	6953	54251
pH	7.11	9.95	5.77
Element			
Al	2.653E-15	2.090E-08	6.065E-09
B	5.930E-03	1.954E-01	9.944E-03
Ba	1.024E-07	2.582E-11	6.806E-07
Ca	1.012E-06	4.605E-06	2.089E-03
Cl	2.014E-04	2.014E-04	2.014E-04
Cr	2.570E-03	1.050E-01	9.430E-02
F	1.878E-05	8.715E-03	5.595E-08
Fe	1.313E-12	4.173E-12	7.278E-12
C	2.584E-04	1.192E+00	4.413E-05
P	1.833E-03	1.586E-04	1.997E-05
K	1.299E-03	1.707E-01	5.159E-03
Li	1.551E-07	6.339E-06	6.915E-06
Mg	8.938E-05	3.125E-06	1.062E-03
Mn	7.306E-14	2.026E-14	5.892E-11
Mo	8.369E-05	3.420E-03	1.260E-04
N	1.942E-04	2.292E-03	2.092E-03
Na	1.365E-02	2.245E+00	6.614E-03
Ni	2.856E-05	3.133E-10	4.424E-02
S	3.353E-03	2.367E-02	4.471E-04
Si	1.867E-04	5.290E-03	5.605E-05
U	1.616E-06	2.171E-02	2.521E-07

Figure 23 shows the predicted concentration of the major WP components, precipitated U minerals, total U in solution, and pH as a function of time during the second stage of Case 10 (n10b1011). Soluble U concentrations are kept at a fairly constant level by formation of schoepite ($UO_3 \cdot 2H_2O$) and $(UO_2)_3(PO_4)_2 \cdot 6H_2O$ (Figure 23 and Table 32). The amount of U in the WP corrosion products also remains nearly constant (Table 31). The pH of the WP solution is kept between 5.6 and 5.9 for most of the second stage of Case 10 by corrosion of 304L and 316L stainless steel WP components (Tables 30 and 32).

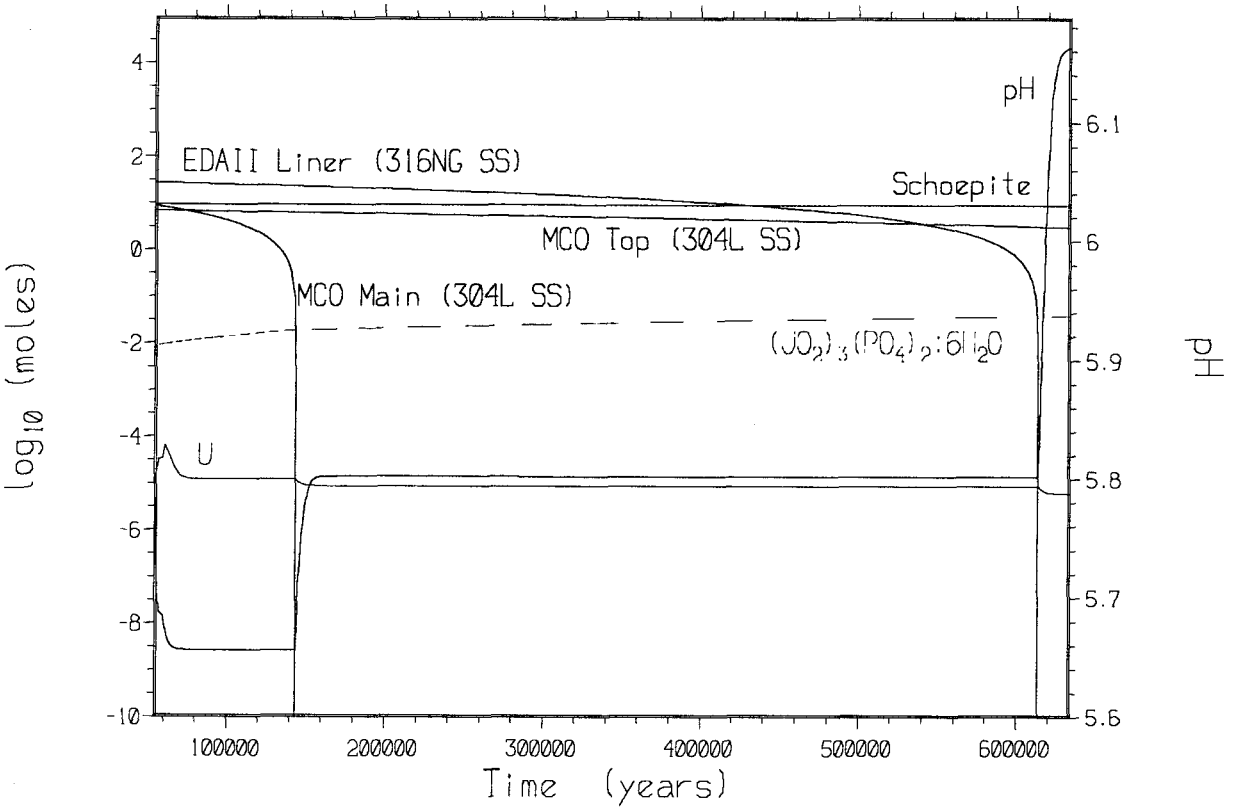

Figure 23. Predicted Concentration of Major Waste Package Components, Precipitated U Minerals, Total U in Solution, and pH as a Function of Time During the Second-Stage of Case 10 (n10b1011)

Table 30. Predicted Mass Remaining of N-Reactor (U-metal) SNF WP Components in Selected Years for the Second-stage of Case 10 (n10b1011)

Years	54250	103210	350290	634080
WP Component	**Mass (kg)**	**Mass (kg)**	**Mass (kg)**	**Mass (kg)**
EDAII Liner (316L SS)	12024	10972	5665	0
MCO Main Canister and Basket (304L SS)	3781	1720	0	0
MCO Top (304L SS)	2986	2844	2130	1311
Mark IA Fuel (outer rod)	6382	0	0	0
Mark IA Fuel (inner rod)	3227	0	0	0
Al 1100 Spacer	91	0	0	0

Source: "Nreactor_U.xls" sheet "Reactant Losses" (Attachment III)

Table 31. Predicted Elemental Composition of Corrosion Products (kg), Total Mass (kg) and Density in Selected Years for the Second Stage of Case 10 (n10b1011)

Years	103210	350290	634080
Element			
O	7.757E+03	1.013E+04	1.213E+04
Al	1.341E+02	1.341E+02	1.341E+02
Ba	8.700E+00	8.662E+00	8.621E+00
Ca	1.356E+01	1.773E+01	2.313E+01
Cl	2.402E-14	0.000E+00	1.894E-13
Cr	3.294E+00	3.279E+00	3.264E+00
Cu	2.087E+02	1.991E+02	1.910E+02
F	8.393E-13	0.000E+00	6.565E-12
Fe	5.714E+03	1.083E+04	1.509E+04
H	1.897E+02	1.908E+02	1.919E+02
C	3.720E-12	0.000E+00	1.539E-11
P	3.777E+00	7.274E+00	1.021E+01
K	4.101E+01	3.262E+01	2.966E+01
Li	5.403E-17	2.008E-19	2.260E-15
Mg	3.225E+01	3.279E+01	3.360E+01
Mn	1.308E+02	2.856E+02	4.153E+02
Mo	1.189E+01	8.880E-16	9.737E-14
N	2.868E-12	0.000E+00	1.337E-12
Na	4.558E-14	0.000E+00	1.970E-12
Ni	2.352E+02	1.924E+02	1.711E+02
S	7.340E-13	7.420E-18	8.592E-12
Si	1.314E+03	1.395E+03	1.469E+03
U	9.609E+03	9.608E+03	9.607E+03
Total (kg)	2.541E+04	3.308E+04	3.951E+04
Density (g/cm^3)	4.472	4.610	4.685

Table 32. Predicted Solution Elemental Composition (mole kg^{-1}) and pH in Selected Years for the Second Stage of Case 10 (n10b1011)

Years	103210	350290	634080
pH	5.66	5.80	6.16
Element			
Al	2.550E-06	1.393E-06	2.631E-07
B	1.239E-05	1.239E-05	1.239E-05
Ba	8.849E-07	7.121E-07	6.262E-07
Ca	8.249E-05	5.880E-06	3.179E-05
Cl	2.014E-04	2.014E-04	2.014E-04
Cr	1.564E-01	5.386E-02	7.056E-03
Cu	8.403E-04	3.212E-04	3.642E-05
F	1.148E-04	1.148E-04	1.148E-04
Fe	9.520E-12	6.521E-12	3.068E-12
C	4.100E-05	4.558E-05	5.954E-05
P	2.354E-08	2.674E-08	4.162E-08
K	1.008E-03	2.775E-04	6.977E-04
Li	6.915E-06	6.915E-06	6.915E-06
Mg	4.006E-05	3.080E-06	1.827E-05
Mn	1.169E-10	4.454E-11	4.970E-12
Mo	4.581E-03	3.731E-03	1.478E-06
N	3.305E-03	1.301E-03	2.795E-04
Na	1.992E-03	1.992E-03	1.992E-03
Ni	8.781E-02	3.344E-02	3.720E-03
S	6.061E-04	3.435E-04	2.096E-04
Si	6.802E-05	7.386E-05	6.097E-05
U	1.231E-05	8.877E-06	6.275E-06

Figure 24 shows the predicted partitioning of U during and shortly after degradation of the N Reactor Mark IA SNF in the second stage of Case 10. Complete degradation of the SNF is predicted to occur by the end of the first year of the second stage. The pH of the WP solution is suppressed slightly by SNF dissolution. Predicted soluble U concentration is kept at a fairly constant level by formation of schoepite ($UO_3 \cdot 2H_2O$) and $(UO_2)_3(PO_4)_2 \cdot 6H_2O$.

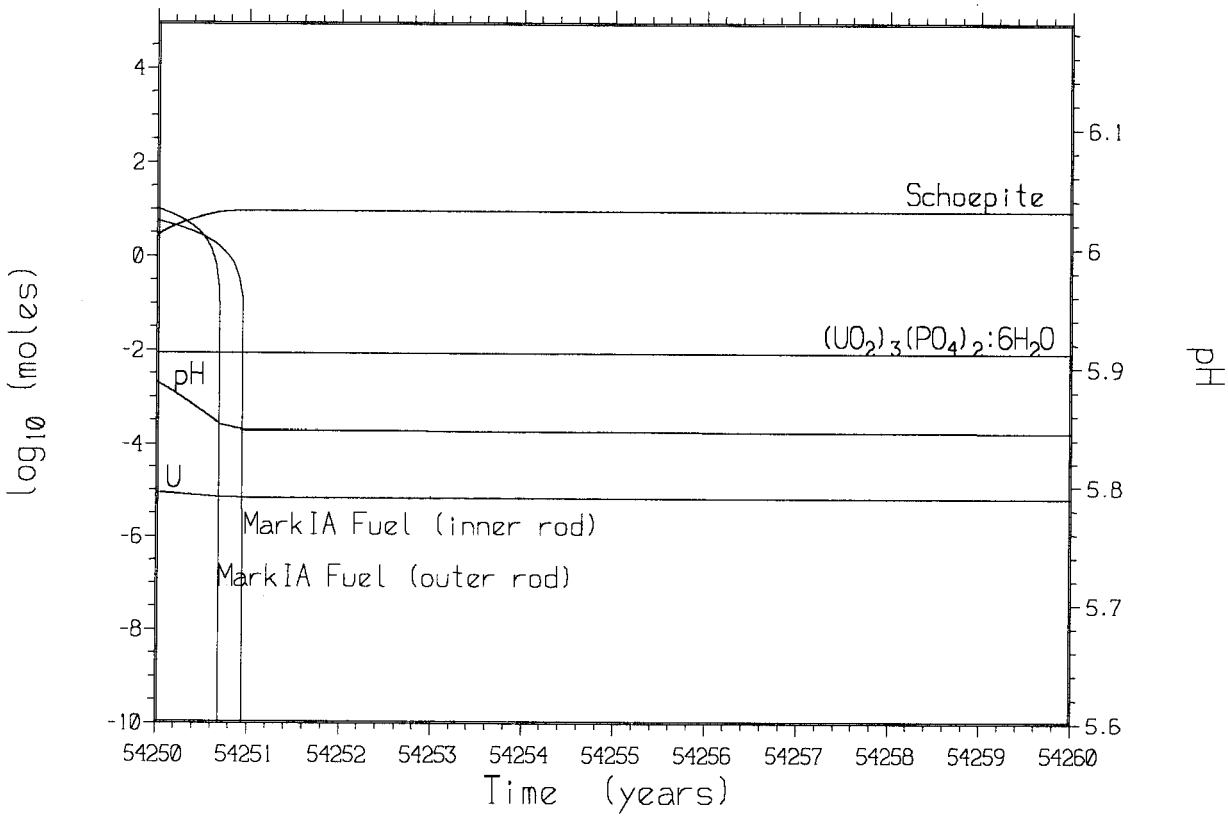

Figure 24. Predicted Concentration of N-Reactor SNF, Precipitated U Minerals, Total U in Solution, and pH as a Function of Time Early in the Second-Stage of Case 10 (n10b1011)

6. RESULTS

This document may be affected by technical product input information that requires confirmation. Any changes to the document that may occur as a result of completing the confirmation activities will be reflected in subsequent revisions. The status of the technical product input information quality may be confirmed by review of the DIRS database.

A principle objective of this calculation was to assess the chemical characteristics that might lead to the retention of U, Pu, and Np in a WP containing N Reactor (U-metal) SNF and HLW glass. Ten EQ6 reaction path calculations were carried out to assess the specific and coupled effects of SNF degradation, steel corrosion, HLW glass degradation, and fluid influx rate on U, Pu and Np mobilization. Corrosion product accumulation (primarily of iron oxide and smectite) and U, Pu, and Np mobilization were examined as well.

In these calculations the geochemical reaction takes place in the waste package solution maintained at a constant volume by steady inflow (drip rate) of fluid having the composition of J-13 well water and by removal of waste package solution at an equal rate. The composition of the waste package solution was determined by chemical reaction of the ions in solution, the elements released by the degradation of the initial waste package internal componenets, the minerals already precipitated, and by the mixing of the in-flowing fluid.

Case 10, the two-stage run, predicted that all of the U in the HLW glass (1.10% of the total U in the WP) would be lost from the WP for conditions of average steel, high HLW glass degradation rates and low drip rate simulated by the first stage of the run. Only 0.02% of the total U in the WP (from Mark IA SNF only) was predicted to be lost during the conditions simulated by the second stage of Case 10, with low steel, average SNF degradation rates, and low drip rate.

Cases 2 and 5 had predicted total U losses from the WP of close to 1%. Both these cases simulated conditions of high steel, average fuel, and low glass degradation rates, with a low drip rate.

Predicted loss of U from the WP was very low (0-0.16%) for the rest of the cases shown in Table 8.

Case 9 was run assuming a decayed composition for N Reactor Mark IA SNF (Table 2). Although predicted total loss of U was very low for this case (0.02%), predicted total loss of Np was high (~83%), and predicted total loss of Pu was low (<2%).

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8. ATTACHMENTS

Attachment I Documentation for Software Routine: volarea (32 pages)

Attachment II. Listing of Files on Compact Disk (5 pages)

Attachment III. One Compact Disk

KL 2/27/01

OFFICE OF CIVILIAN RADIOACTIVE WASTE MANAGEMENT
SPECIAL INSTRUCTION SHEET

1. QA: QA

Complete Only Applicable Items

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2. Record Date	3. Accession Number
02/01/2001	ATT-TO MOL.20010227.0017
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6. Title
EQ6 CALCULATIONS FOR CHEMICAL DEGRADATION OF N REACTOR (U-METAL) SPENT NUCLEAR FUEL WASTE PACKAGES

7. Document Number(s)	8. Version
CAL-EDC-MD-000010	REV 00
9. Document Type	**10. Medium**
DATA	CD-ROM

11. Access Control Code
PUB

12. Traceability Designator
DC #26528

13. Comments
THIS IS A SPECIAL PROCESS CD/ROM ENCLOSED AS PART OF ATTACHMENT III, AND CAN BE LOCATED THROUGH THE RPC

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OFFICE OF CIVILIAN RADIOACTIVE WASTE MANAGEMENT
ELECTRONIC SOURCE FILE VERIFICATION

QA: N/A

DOCUMENT TITLE:

EQ6 Calculations for Chemical Degradation of N Reactor (U-metal) Spent Nuclear Fuel Waste Packages

2. DOCUMENT IDENTIFIER:	3. REVISION DESIGNATOR:
CAL-EDC-MD-000010	REV 00

ELECTRONIC SOURCE FILE INFORMATION

4. ELECTRONIC SOURCE FILE NAME WITH FILE EXTENSION PROVIDED BY THE SOFTWARE:
N-Reactor00.doc

5. DATE LAST MODIFIED:	6. ELECTRONIC SOURCE FILE APPLICATION: (I.E., EXCEL, WORD, CORELDRAW)	7. FILE SIZE IN KILOBYTES:
1/31/01	Word	5435 KB

8. FILE LINKAGE INSTRUCTIONS/INFORMATION:
N/A

9. FILE CUSTODIAN: (I.E., DC, OR DC APPROVED CUSTODIAN)	10. FILE LOCATION FOR DC APPROVED CUSTODIAN: (I.E., SERVER, DIRECTORY)
DC	DC

11. PRINTER SPECIFICATION (I.E., HP4SI) INCLUDING POSTSCRIPT INFORMATION (I.E., PRINTER DRIVER) AND PRINTING PAGE SETUP: (I.E., LANDSCAPE, 11 X 17 PAPER)
HP5Mc (color printer) - portrait 8½" x 11"

12. COMPUTING PLATFORM USED: (I.E., SUN)	13. OPERATING EQUIPMENT USED: (I.E., UNIX, SOLARIS)
PC	Windows

14. ADDITIONAL HARDWARE/SOFTWARE REQUIREMENT USED TO CREATE FILE(S):	15. ACCESS RESTRICTIONS: (IF ANY)
N/A	N/A

COMMENTS/SPECIAL INSTRUCTIONS

16.
N/A

The Electronic Source File (ESF) for the approved (on one CD) document and attachment III (on one CD) was submitted by the author and was hand carried to DCC, 02-05-01 by EDC Personnel

CERTIFICATION

17. NAME (Print and Sign)			18. DATE:
Patricia A Bernot			1/31/01
19. ORGANIZATION:	**20. DEPARTMENT:**	**21. LOCATION/MAILSTOP:**	**22. PHONE:**
SAIC/M&O	Waste Package	423	(702) 295-3215

DC USE ONLY

23. DATE RECEIVED:	24. DATE REVIEWED:	25. DATE FILES TRANSFERRED:
2-5-01	2/21/2001	02-07-2001
26. NAME (Print and Sign):		**27. DATE:**
Teri M. McCoy		2/21/2001

ATTACHMENT I. DOCUMENTATION FOR SOFTWARE ROUTINE: VOLAREA

1. Listing of volarea (volarea.c on Attachment III)

```
/*volarea.c The purpose of this program is to calculate volumes and areas
  of shapes inside a waste package, and total those parameters for each
  material.  This program operates stand alone to support the description
  of materials in the waste package; it also operates as the central part
  of the program eqsetup.c, which provides the input files for EQ6.  In
  calculating the areas of prism and cylinder shells, the small area at the
two
  ends, between the principal surfaces is not included. The program also
  calculates the moles of these shapes, according to composition and
  atomic weights.  The moles and grams are also broken down by elements
  (which are called components, in keeping with EQ3/6 terminology).
  All the input is checked for consistency, except the number of components
  (elements) in each material.  This program was initially developed before
    eqsetup.c, but the present version ultimately evolved as a reduction from
    eqsetup.c (for which the calculations for several of the more complex
    shapes were expanded and corrected).  In eqsetup.c the seperate printing
    of areas and volumes was for checking purposes only, hence the name of the
    file pointer in which they are printed, ferr.

  The atomic weights are read in from the file atwts.in, using the subroutine
  bldatwts().  The elements use their international chemical symbols, with
the
  first letter capitalized.  The individual element weight values are for the
  natural isotopic mixture, except for Pu, which uses only the Pu-239 value,
and
  U, for which the principal isotopes of interest, (233, 235, 238, etc)
  can be entered individually (e.g. U-233, etc).  These isotopic designations
  cannot be used in the present version of EQ3/6, so they are combined into
  a single element with symbol "U" having an average atomic weight calculated
  from the isotopic composition for that material.  Two, or more, materials
  having different U isotope compositions will give slightly different
  molecular weights, but that doesn't matter because EQ3/6 uses its own value
  for atomic weight.  The only parameters fed to EQ3/6 are moles remaining
  and molar volume, and this procedure ensures that they will be calculated
  in a consistent manner.  For this system to work, all of the
  uranium isotopes must appear at the end of the material component list, but
  they may appear in any order.  If the U isotopes are not confined to the
  end of the list, the program will quit with an appropriate error message.

  The input, data.in, is read into an array of lines. This array is processed
as
  blocks of shapes, materials, and structures.  The structures are built from
  shapes. Total mass and area are accumulated by traceing the shapes through
  their occurrences in the hierarchy of structures.  Since each shape is
  associated with a single material (mtrl[i]) the mass and area of each
material
  can be accumulated along with accumulation for shapes.  The principal
results
  of this process are the surface areas and moles for each material (the
latter
  being computed from the total mass for the material and its molecular
weight),
  since this is the primary input to EQ3/6.  The shape components of a
```

```
  structure have one line each.  Each shape component line starts with the
keyword
  component, followed by an equal sign and two fields.  The first field is
the
  name of the shape; the second field is the number of times the shape occurs
in
  the structure.  If this number is negative, the area and volume of the
shape
  will be subtracted instead of added.  This capability can be used to remove
  surfaces that are double counted when a solid structure is built of
  elementary shapes (such as a cone on top of a cylinder).  Such a removal
  would be accomplished by subtracting a very thin plate having the surface
  area to be removed, but only an infinitessimal volume.

  Areas for each material are accumulated in the routine bldmoles() for
  convenience.  The area calculation incorporates a fracture factor, which
can
  account for additional area due to internal fracturing, or for reduced
exposed
  area due to protection such as intact cladding.  Bookkeeping for these
  factor values is by shape.  The designator in the file data.in is
  fracture_factor; for internal fracturing fracture_factor > 1; for
simulating
  the protection by partly intact cladding fracture_factor < 1, and the value
  is inversely proportional to the amount of cladding protection left (which
  decreases with time).

  There are two different forms for comments: (1) Anything after the
obligatory
  fields in a keyword statement;  (2) Any line that begins below with an '*'.
  The former are copied into the input array of lines, but not read because
  each keyword keys a read of only a limited number of fields.  The latter
  are simply diverted into the debugging file, "junk.out".

  The input file, "data.in" also has a capability like the FORTRAN namelist,
  provided that the variable name is preceded by a character less than
  ASCII 48 (decimal) and then a code line for reading that variable is
  inserted at an appropriate place in the program.  This capability is
  presently implemented for the global variable literswater, for which a
  nominal value is assigned in the program, but which may be overridden
  by reading in the function bldmoles().  It is also implemented for the
local
    (to the subroutine bldmoles()) variable totalvolume, for which there is
    no default value because the parameter is not used at all if there is
    no namelist type input for it.  For literswater the overriding value will
    be read if it occurs on any line of "data.in" provided the variable name
  (literswater) is prefixed by '$'.  If totalvolume is input, literswater
    will be calculated as the difference between the value of totalvolume (in
    liters) and the total volume of all the shapes (or all the materials) in
    the waste package.

  The areas and volumes of the individual shapes are calculated in the
    subroutine buildvals(). The input parameters for each shape are
    straightforward, except for the spherical segment, which uses the
    parameters: sphereseg, altitude, largerad, smallrad.  The use of the
    shape parameters is evident from the formulae for each shape in the
    switch statement of the subroutine bldvals().
```

```
  */

#include <stdio.h>
#include <float.h>
#include <string.h>
#include <stdlib.h>
#include <math.h>
#define PI (float)acos(-1)
#define MAXLOOP 100//max steps in trace of a shape through structure
hierarchy

//In the following array definitions i refers to the first index; j to the
second
FILE *fin,*ferr;
float findfloat(char*,int,int);//gets a float number from an array of strings
int findatwtindx(char*);//finds the index of an element in the atomic wt
table
float areas[100], //areas of individual shapes
     volumes[100],//volumes of individual shapes
      densities[100],//densities of individual materials
      degrates[100],//degradation rates of individual materials
      gramvals[30][30],//wt fraction of element j in material i
      compvals[30][30];//mole fraction of element j in material i
float mass[100]={0},//accumulates mass of material i
      mareas[20]={0},//accumulates area of material i
       literswater=3937,//water in bathtub, may be overridden in bldmoles().
       totalvolume,
       atwts[100],//array of atomic weights (read from atwts.in)
       nmoles[100]={0};//moles of material i
float bldmolwt(int),//builds molecular weight for each material
      mvolumes[20],//volume of a gram mole of material i
       fudgefac[20],//simply goes into EQ3/6 input; not now used for anything
       temperature=25,//selects thermo libriary for EQ3/6
       fracfac=1;//fracture factor for glass; should be an array for
additional mtrl
void etrim(char*),//trims blanks from end of a string
      ftrim(char*),//trims blanks from the beginning of a string
       errproc(char*,char*),//outputs two strings describing the error and
exits
       bldmoles(),//builds total masses and volumes for each material and
shape
       bldatwts();//builds the atomic weights array from atwts.in
char lines[800][100];  //array of input lines
char Uxnames[5][3]={"Ua","Ub","Uc","Ud","Ue"};//dummy names for U
combinations
        //used internally; EQ3/6 reads only U for uranium.
float mwtUxvals[5]={0};//Average atomic wt for all the U isotopes in this
mtrl
int numUwts=0;//Counts the number of materials with multiple U isotopes
char mtrl[100][20],//name of material for shape i
     compnames[30][30][20],//name (symbol) of element j of material i
      matnames[100][20],//name of material i
      shapenames[100][20];//name of shape i
int buildvals(int,int),//builds array of lines from the input file, data.in
     numshapes=0,//number of shape blocks read from the lines array
      nummaterials=0,//number of material  blocks read
      numstructures=0,//accumulates number of structures read from data.in
```

```
     get1of3(char*,char*,char*,int);//identify 3 basic input block types
(data.in)
int mindex=0,//tracks index for material block currently being read
   sindex=0,//tracks index for shape block currently being read
    findint(char*,int,int),//returns integer parameter when keyword is found
    findstr(char*,char*,int,int),//copies string parameter when keyword is
found
  stype[100],//shapetype for shape i
    ttype[100],//solid or shell for shape i
    occrrncs[100]={0},//lowest level occurrences for shape i (from data.in)
    compnums[100],//number of elements in material i
    numlines,//number of lines read from data.in
    get2(char*,char*,char),//splits a string at the third argument
    numelements,//number of elements read from atwts.in
    dislaw=3,//dissolution law index; simply passed to EQ3/6
    plaw=0,//precipitation law index; simply passed to EQ3/6
    loopcount;//counts steps in traceing a shape through the structure
hierarchy
char atnames[120][7]; //to be read from atwts.in, large to permit isotopes
char stnames[25][20],        //array of structure names
     subnames[25][20][20];   //array of substructure names within structure
int nstoccrrncs[25]={0},  //number of occurrences for this structure
    nsuboccrrncs[25][20]={{0}}, //number of this substructure occurrences
     numsubs[25];         //number of substructures in this structure
int getcomps(int,char*); //returns num occurrences of this component in
structure
float atwts[100],//array of atomic weights
    afcone(float,float,float),//calculates area of the frustrum of a cone
     vfcone(float,float,float);//calculates volume of the frustrum of a cone
float matvolume[100]={0},//accumulates total volume of material i
    smass[100]={0},//accumulates total mass for all occurrences of shape i
     sarea[100]={0},//accumulates total area for all occurrences of shape i
     svolume[100]={0};//accumulates total volume for all occurrences of shape
i
int calcoccrrncs(char*),//calc number of occurrences of a shape or structure
    foundc; //used as BOOL for occurrence of a shape

void main()
{int i=0,key;
char dummy[100];
for(i=0;i<20;i++)fudgefac[i]=1;//nominal value for unused parameter
bldatwts();//read table of atomic weights
if((fin=fopen("data.in","r"))==NULL)
  {printf("couldn't open input\n");
  exit(0);}
ferr=fopen("data.out","w");
i=0;   //the following line converts data.in to an internal array (lines[])
while((fgets(dummy,100,fin)!=NULL)&&(i<800))
  {if(dummy[0]=='*') fprintf(ferr,"%s",dummy);//divert comment to the output
  else strcpy(lines[i++],dummy);}
numlines=i;
i=0;   //the following lines copy non-comment lines of data.in into lines[]
while((fgets(dummy,90,fin)!=NULL)&&(i<700))
  {if(dummy[0]=='*') fprintf(ferr,"%s",dummy);//divert comment to the output
  else strcpy(lines[i++],dummy);}
i=0;//The following loop builds a data array for each shape, material,
structure
```

```
while (i<=numlines)
  {while((lines[i][0]<48)&&(i<numlines))i++;//readthrough blank lines and any
                                           //namelist items
  if(i>=numlines)break;
  if((key=get1of3("shape","material","structure",i))==0)//type of block
     errproc("shape or material or structure",lines[i]);
  i+=buildvals(key,i);}//build array for this block
bldmoles();//comprehensive calculations of areas and volumes
printf("BY SHAPE\n");//diagnostic print to screen and file
fprintf(ferr,"BY SHAPE\n");
for(i=0;i<numshapes;i++)
  {printf("%s Area=%f Volume=%f Material=%s\n",
              shapenames[i],sarea[i],svolume[i],mtrl[i]);
  fprintf(ferr,"%s Area=%f Volume=%f Material=%s\n",
              shapenames[i],sarea[i],svolume[i],mtrl[i]);}
printf("\nBY MATERIAL\n");
fprintf(ferr,"\nBY MATERIAL\n");
for(i=0;i<nummaterials;i++)
  {printf("%s Density=%g Moles=%g Area=%g Volume=%g\n",
        matnames[i],densities[i],nmoles[i],mareas[i],matvolume[i]);
  fprintf(ferr,"%s Density=%g Moles=%g
    Area=%g Volume=%g\n",
        matnames[i],densities[i],nmoles[i],mareas[i],matvolume[i]);}
printf("%d input lines read\n",numlines);}



//Determines  if line i starts a block of one of the 3 types
int get1of3(char *s1,char *s2,char *s3,int i)
{int j;
char *p,stag[20];
if((p=strchr(lines[i],'='))==NULL) return 0;
j=(int)(p-lines[i]);
strncpy(stag,lines[i],j);
stag[j]='\0';
etrim(stag);
if(strcmp(s1,stag)==0) return 1;
else if (strcmp(s2,stag)==0) return 2;
else if (strcmp(s3,stag)==0) return 3;
else return 0;}


//Builds data array for each block of data.in, including calculation of
//volume and surface area for each shape.
int buildvals(int type,int row)
{int i=1,j,numgrp,k;//number of lines in this block/group
char tempstr[100],stag[20];//to hold substrings for further processing
float x,y,z,r,t,t1,t2,f,a,turns,dr,r1,r2;//for shape dimensions
while((get1of3("shape","material","structure",row+i)==0)&&(lines[row+i][0]>=4
8)&&
    (row+i<=numlines))i++;   //find number of lines in this block
numgrp=i;//number of lines in this group/block
strcpy(tempstr,lines[row]);
if(type==2) //build array for this material block
  {get2(stag,tempstr,'=');
  strcpy(matnames[mindex],tempstr);
  if((densities[mindex]=findfloat("density",row,numgrp))==0)
```

```
            errproc("no density for ",tempstr);
  if((j=findstr(stag,"degrate",row,numgrp))==0)
            errproc("no degradation rate for ",tempstr);
  strcpy(tempstr,lines[row+j]);
  i=get2(stag,tempstr,'=');
  strcpy(tempstr,lines[row+j]+i+1);
  if((k=get2(stag,tempstr,' '))==-1)
        errproc("missing degrate units for ",matnames[mindex]);
  degrates[mindex]=(float)atof(stag);
  if(strcmp(tempstr,"moles")==0)degrates[mindex]*= -1;//flag for alternate
units
  else if (strcmp(tempstr,"grams")!=0)                //used in bldmoles
    errproc("invalid name for degradation rate units for ",matnames[mindex]);
  if((compnums[mindex]=findint("numelements",row,numgrp))==0)
            errproc("no component number for ",tempstr);
  if(compnums[mindex]+3>numgrp)
    {printf("compnums=%d  numgrp=%d  nummtrls=%d\n",
                    compnums[mindex],numgrp,nummaterials);
     errproc("too many lines",tempstr);}
  for(j=0;j<compnums[mindex];j++)  //elements must be last
    {strcpy(tempstr,lines[row+4+j]);  //four lines for the previous items
    get2(stag,tempstr,'=');
    strcpy(compnames[mindex][j],stag);
   gramvals[mindex][j]=(float)atof(tempstr)/100;
   compvals[mindex][j]=
       gramvals[mindex][j]/atwts[findatwtindx(compnames[mindex][j])];}
  mindex++; //processing for this material completed
  nummaterials++;}
else if(type==1)//processing for a shape block
  {get2(stag,tempstr,'=');
  strcpy(shapenames[sindex],tempstr);
  if((j=findstr(stag,"type",row,numgrp))==0) errproc("no type for
shape",tempstr);
  strcpy(tempstr,lines[row+j]);
  i=get2(stag,tempstr,'=');
  strcpy(tempstr,lines[row+j]+i+1);
  get2(stag,tempstr,' ');
  if(strcmp(stag,"cube")==0) stype[sindex]=0;
  else if(strcmp(stag,"box")==0) stype[sindex]=1;
  else if(strcmp(stag,"cylinder")==0) stype[sindex]=2;
  else if(strcmp(stag,"sphere")==0) stype[sindex]=3;
  else if(strcmp(stag,"rtprism")==0) stype[sindex]=4;
  else if(strcmp(stag,"etprism")==0) stype[sindex]=5;
  else if(strcmp(stag,"hprism")==0) stype[sindex]=6;
  else if(strcmp(stag,"helix")==0) stype[sindex]=7;
  else if(strcmp(stag,"conefrustrum")==0) stype[sindex]=8;
  else if(strcmp(stag,"sphereseg")==0) stype[sindex]=9;
  else if(strcmp(stag,"pie")==0) stype[sindex]=10;
  else errproc("No shape type ",stag);
  if(strcmp(tempstr,"shell")==0) ttype[sindex]=0;
  else ttype[sindex]=1;
  occrrncs[sindex]=findint("occurrences",row,numgrp);//returns zero if the
                                                     //shape occurs in a structure
  if(findstr(stag,"matname",row,numgrp)==0) //material for this shape
     errproc("no material for shape",shapenames[sindex]);
  strcpy(mtrl[sindex],stag);
  if((x=findfloat("fracture_factor",row,numgrp))>0) fracfac=x;
```

```
  else fracfac=1;
  switch(stype[sindex])//get the appropriate dimensions for this shape
                       //and calculate its area and volume
  {case 0:                                          //cube
      if((x=findfloat("side",row,numgrp))==0)errproc("no side for ",stag);
       if(ttype[sindex]==1)  //for solid
         {areas[sindex]=6*(float)pow(x,2);
         areas[sindex]*=fracfac;
         volumes[sindex]=(float)pow(x,3);}
       else                  //for shell
         {if((t=findfloat("thickness",row,numgrp))==0)
             errproc("no thickness for cube shell","");
         areas[sindex]=6*(float)((pow(x,2)+pow(x-2*t,2)));
         areas[sindex]*=fracfac;
         volumes[sindex]=(float)((pow(x,3)-pow(x-2*t,3)));}
       break;
    case 1:                                         //rectangular box
      if((x=findfloat("side1",row,numgrp))==0)errproc("no side1 for ",stag);
      if((y=findfloat("side2",row,numgrp))==0)errproc("no side2 for ",stag);
      if((z=findfloat("side3",row,numgrp))==0)errproc("no side3 for ",stag);
       if(ttype[sindex]==1)
         {areas[sindex]=2*(x*y+y*z+x*z);
         areas[sindex]*=fracfac;
         volumes[sindex]=x*y*z;}
      else
         {if((t=findfloat("thickness",row,numgrp))==0)
             errproc("no thickness for box shell","");
         areas[sindex]=2*(x*y+y*z+x*z)
             +2*(float)((x-2*t)*(y-2*t)+(y-2*t)*(z-2*t)+(z-2*t)*(x-2*t));
         areas[sindex]*=fracfac;
        volumes[sindex]=x*y*z-(x-2*t)*(y-2*t)*(z-2*t);}
       break;
    case 2:                                        //cylinder
      if((r=findfloat("radius",row,numgrp))==0)errproc("no radius for
",stag);
      if((z=findfloat("length",row,numgrp))==0)errproc("no length for
",stag);
       if(ttype[sindex]==1)
         {areas[sindex]=2*PI*r*z+2*PI*r*r;
         areas[sindex]*=fracfac;
         volumes[sindex]=PI*r*r*z;}
      else
         {if((t=findfloat("thickness",row,numgrp))==0)
             errproc("no thickness for cylinder shell","");
         areas[sindex]=2*PI*r*z+2*PI*(r-t)*z;
         areas[sindex]*=fracfac;
        volumes[sindex]=PI*r*r*z-PI*(r-t)*(r-t)*z;}
       break;
   case 3:                              //sphere
      if((r=findfloat("radius",row,numgrp))==0)errproc("no radius for
",stag);
       if(ttype[sindex]==1)
         {areas[sindex]= 4*PI*r*r;
         areas[sindex]*=fracfac;
         volumes[sindex]=4*PI*r*r*r/3;}
      else
         {if((t=findfloat("thickness",row,numgrp))==0)
```

```
            errproc("no thickness for spherical shell","");
          areas[sindex]=4*PI*(r*r+(r-t)*(r-t));
          areas[sindex]*=fracfac;
         volumes[sindex]=4*PI*r*r*r/3-4*PI*(r-t)*(r-t)*(r-t)/3;}
        break;
    case 4:                              //isoceles right triangle prism
      if((x=findfloat("side",row,numgrp))==0)errproc("no side for ",stag);
      if((z=findfloat("length",row,numgrp))==0)errproc("no length for
",stag);
      f=2+(float)sqrt(2);      // also 1+cot(22.5deg)
       if(ttype[sindex]==1)
         {areas[sindex]=x*f*z+x*x; //area of sides and ends
         areas[sindex]*=fracfac;
         volumes[sindex]=x*x*z/2;}
      else
         {if((t=findfloat("thickness",row,numgrp))==0)
             errproc("no thickness for right triangle prism shell","");
         areas[sindex]=x*f*z+(x-f*t)*f*z;
         areas[sindex]*=fracfac;
        volumes[sindex]=(x*x-(x-f*t)*(x-f*t))*z/2;}
       break;
    case 5:                              //equilateral triangle prism
      if((x=findfloat("side",row,numgrp))==0)errproc("no side for ",stag);
      if((z=findfloat("length",row,numgrp))==0)errproc("no length for
",stag);
       if(ttype[sindex]==1)
         {areas[sindex]=3*x*z+x*x*(float)sqrt(3)/2; //area of sides and ends
         areas[sindex]*=fracfac;
         volumes[sindex]=x*x*z*(float)sqrt(3)/4;}
      else
         {if((t=findfloat("thickness",row,numgrp))==0)
             errproc("no thickness for equilateral triangle prism shell","");
        f=2*(float)sqrt(3);      // also 2cot(30deg)
         areas[sindex]=3*x*z+3*(x-f*t)*z;
         areas[sindex]*=fracfac;
        volumes[sindex]=x*x*z*(float)sqrt(3)/4-(x-f*t)*(x-
f*t)*z*(float)sqrt(3)/4;}
       break;
    case 6:                              //hexagon based prism
      if((x=findfloat("side",row,numgrp))==0)errproc("no side for ",stag);
      if((z=findfloat("length",row,numgrp))==0)errproc("no length for
",stag);
       if(ttype[sindex]==1)
         {areas[sindex]=6*x*z+3*x*x*(float)sqrt(3); //area of sides and ends
         areas[sindex]*=fracfac;
         volumes[sindex]=6*x*x*z*(float)sqrt(3)/4;}
      else
         {if((t=findfloat("thickness",row,numgrp))==0)
             errproc("no thickness for hexagonal prism shell","");
        f=2/(float)sqrt(3);      // also 2tan(30deg)
         areas[sindex]=6*x*z+6*(x-f*t)*z;
         areas[sindex]*=fracfac;
        volumes[sindex]=6*x*x*z*(float)sqrt(3)/4
                        -6*(x-f*t)*(x-f*t)*z*(float)sqrt(3)/4;}
       break;
    case 7:                              //helix
      if((turns=findfloat("turns",row,numgrp))==0)
```

```
                    errproc("no turns for ",stag);
      if((a=findfloat("smallradius",row,numgrp))==0)
                    errproc("no smallradius for ",stag);
      if((r=findfloat("largeradius",row,numgrp))==0)
                    errproc("no largeradius for ",stag);
      if((z=findfloat("altitude",row,numgrp))==0)errproc("no altitude for
",stag);
       if(ttype[sindex]==1)
         {areas[sindex]=2*PI*a*(float)sqrt(z*z+pow(2*PI*r*turns,2));
         volumes[sindex]=areas[sindex]*a/2;
         areas[sindex]*=fracfac;}  //now adjust area for fractures
      else errproc("no helical shell","");
       break;
/* Alternative area=PI*a*z/sin(alph), where alph is the dihedral angle
between
   the horizontal and any tangent plane of the helix.  This formulation would
    require only 3 input parameters.*/

    case 8:                          //frustum of cone
      if((z=findfloat("altitude",row,numgrp))==0)errproc("no altitude for
",stag);
      if((r1=findfloat("bottomrad",row,numgrp))==0)
                        errproc("no bottom radius for ",stag);
      if((r2=findfloat("toprad",row,numgrp))==0)
                        errproc("no top radius for ",stag);
       if(ttype[sindex]==1)
         {areas[sindex]=afcone(r1,r2,z);
         areas[sindex]*=fracfac;
         volumes[sindex]=vfcone(r1,r2,z);}
      else
         {if((t=findfloat("thickness",row,numgrp))==0)
             errproc("no thickness for cone frustrum shell","");
        dr=t*(float)sqrt(1+pow(r1-r2,2)/z/z);
         areas[sindex]=afcone(r1,r2,z)+afcone(r1-dr,r2-dr,z);
       areas[sindex]-=PI*(r2*r2+r1*r1);//remove top and bottom from outer
        areas[sindex]-=PI*(float)(pow(r2-dr,2)+pow(r1-dr,2));//and from inner
         areas[sindex]*=fracfac;
        volumes[sindex]=vfcone(r1,r2,z)-vfcone(r1-dr,r2-dr,z);}
       break;
   case 9://segment of a sphere; large and small radii of the segment (r1,r2)
          //are meassured from an axis of the sphere; the radius of the
           //actual sphere is derived from r1,r2, and the altitude, z. For a
           //shell, the thickness, t, is for the material itself.  The
           //projections of this thickness onto the large and small segment
           //planes are derived as the variables t1,t2.
      if((z=findfloat("altitude",row,numgrp))==0)//distance between top *
bottom
                        errproc("no altitude for ",stag);
        if((r1=findfloat("largerad",row,numgrp))==0)
                        errproc("no largerad for ",stag);
      if((r2=findfloat("smallrad",row,numgrp))==0)
                        errproc("no smallrad for ",stag);
      r=(float)sqrt(r2*r2+pow(r1*r1-r2*r2+z*z,2)/(4*z*z));//radius of sphere
       if(ttype[sindex]==1)
         {areas[sindex]=PI*(2*r*z+r1*r1+r2*r2); //area of upper and lower too
         areas[sindex]*=fracfac;
         volumes[sindex]=PI*z*(z*z+3*(r1*r1+r2*r2))/6;}
```

```
      else
         {if((t=findfloat("thickness",row,numgrp))==0)
             errproc("no thickness for sphere segment shell","");
         t1=t*r/r1;//project thickness onto large plane of segment
         t2=t*r/r2;//onto the small plane of segment
         areas[sindex]=2*PI*(r*z+(r-t)*(z-t));
         areas[sindex]*=fracfac;
        volumes[sindex]=PI*z*(z*z+3*(r1*r1+r2*r2))/6
                    -PI*(z-t)*((z-t)*(z-t)+3*((r1-t1)*(r1-t1)+
                       (r2>t2?(r2-t2)*(r2-t2):0)))/6;}//If the small segement
radius
                       //is less than the projected thickness, it is omitted
from
                       //the volume calculation.  This is the usual
condition,
                       //since the segment is usually a cap.
       break;
   case 10://pie shape;radius, length, angle, calc for solid only
      if((z=findfloat("length",row,numgrp))==0)//distance between top *
bottom
                         errproc("no length for ",stag);
         if((r=findfloat("radius",row,numgrp))==0)
                         errproc("no radius for ",stag);
      if((a=findfloat("angle",row,numgrp))==0)
                         errproc("no angle for ",stag);
         areas[sindex]=(2*PI*r*r+2*PI*r*z)*(a/360)+2*r*z;
           volumes[sindex]=PI*r*r*z*a/360;}
    sindex++;  //processing for this shape complete
    numshapes++;}
else if (type==3)//build array for this structure
  {get2(stag,tempstr,'=');
  strcpy(stnames[numstructures],tempstr);
  for(i=1;i<numgrp;i++)
    if((j=getcomps(row+i,stag))!=0)
       {nsuboccrrncs[numstructures][numsubs[numstructures]]=j;
        strcpy(subnames[numstructures][numsubs[numstructures]],stag);
       numsubs[numstructures]++;}
  nstoccrrncs[numstructures]=findint("occurrences",row,numgrp);
  numstructures++;}
return numgrp;}

//for a component line of a structure block, returns occurrences
int getcomps(int rw,char* retstr)//duplicates findstr(), but for a single
line
{int i;
char *p,stag[20],tempstr[100];
if(strncmp(lines[rw],"component",9)!=0) return 0;
strcpy(tempstr,lines[rw]);
p=strchr(lines[rw],'=');
i=(int)(p-lines[rw]);
strcpy(tempstr,lines[rw]+i+1);
get2(stag,tempstr,' ');
strcpy(retstr,stag);
return atoi(tempstr);}

float afcone(float rl,float ru,float h) //area of the frustrum of a cone
{float area;
```

```
area=PI*(rl*rl+ru*ru);//top and bottom disks
area+= PI*h*(rl+ru)*(float)sqrt(1+rl*rl*pow(1-ru/rl,2)/h/h);
return area;
}

float vfcone(float rl,float ru,float h) //volume of the frustrum of a cone
{return PI*h*(rl*rl+rl*ru+ru*ru)/3;}

//Find the float numerical value in a statement that begins with the
specified
//keyword (keystr).
float findfloat(char* keystr,int startrow,int numrows)
{int i=0;
char stag[20],tempstr[100];
while ((strncmp(keystr,lines[startrow+i],strlen(keystr))!=0)&&(i<=numrows))
    i++;
if (i==numrows+1) return 0;
strcpy(tempstr,lines[startrow+i]);
get2(stag,tempstr,'=');
return (float)atof(tempstr);}

//Find the int numerical value in a statement that begins with the specified
//keyword (keystr).
int findint(char* keystr,int startrow,int numrows)
{int i=0;
char stag[20],tempstr[100];
while
((strncmp(keystr,lines[startrow+i],strlen(keystr))!=0)&&(i<=numrows))i++;
if (i>=numrows) return 0;
strcpy(tempstr,lines[startrow+i]);
get2(stag,tempstr,'=');
return atoi(tempstr);}

//This function searches for a key at the start of the line and copies the
//string (containing no blanks) following the equal sign into retstr.
//It returns zero if the keystring is not found, otherwise the row in which
found.
//It is analogous to findfloat and findint, but does not return the
//information, since C cannot assign to a character string.
int findstr(char *retstr,char *keystr,int startrow,int numrows)
{int i=0;
char stag[20],tempstr[100];
while
((strncmp(keystr,lines[startrow+i],strlen(keystr))!=0)&&(i<=numrows))i++;
if (i==numrows) return 0;
strcpy(tempstr,lines[startrow+i]);
get2(stag,tempstr,'=');
strcpy(retstr,tempstr);
return i;}

//copies the strings occurring before and after the separator c ('=' or ' ')
int get2(char *stag,char *sdummy,char c)
{int i,index,len;
char *p;
len=strlen(sdummy);
p=strchr(sdummy,c);
i=(int)(p-sdummy);
```

```
index=i;
strncpy(stag,sdummy,i);
stag[i]='\0';
etrim(stag);
strcpy(sdummy,p+1);
i=0;
while((sdummy[i]==' ')&&(i<len))i++;
if((i==len)||(sdummy[i]=='\n')) return -1;//can't find a second word on rt
side
strcpy(sdummy,sdummy+i);
while((sdummy[i]!=' ')&&(sdummy[i]!='\0')&&(sdummy[i]!='\n'))i++;
sdummy[i]='\0';
ftrim(sdummy);
return index;}

void etrim(char *dummy)//trims trailing blanks
{int i;
i=strlen(dummy)-1;
while(dummy[i]<=32)i--;
dummy[i+1]='\0';}

//trims leading blanks
void ftrim(char *dummy)    //use in get2 so that fdummy starts with a non-
blank
{int i=0;
while(dummy[i]<=32)i++;
strcpy(dummy,dummy+i);}

//prints a two string error message
void errproc(char *str1,char *str2)
{printf("%s %s\n",str1,str2);
exit(0);}

//accumulate total mass, area, and volume for shapes[j] and mtrls[i]
void bldmoles()
{int i,j,k,normflag=0;
float x,molwt,checkvol=0,totalvolume,compsum[50]={0};
if((x=findfloat("$literswater",0,numlines))>0) literswater=x;
else if((x=findfloat("$totalvolume",0,numlines))>0)
    {totalvolume=x;
    normflag=1;}
for(i=0;i<nummaterials;i++)
  {checkvol=0;
  for(j=0;j<numshapes;j++)
    if(strcmp(matnames[i],mtrl[j])==0)
          {if((k=occrrncs[j])==0)
             {foundc=0;
            loopcount=0;
              k=calcoccrrncs(shapenames[j]);
            if((foundc==0)||(k==0))errproc("no occurrences for
",shapenames[j]);}
           mass[i]+=volumes[j]*k*densities[i];
           mareas[i]+=areas[j]*k;
           checkvol+=volumes[j]*k;
           smass[j]+=volumes[j]*k*densities[i];
           sarea[j]+=areas[j]*k;
           svolume[j]+=volumes[j]*k;}
```

```
  if(normflag==1)
      {literswater=totalvolume-checkvol;
      fprintf(ferr,"Total solids volume=%.4e Void volume=%.4e\n",
            checkvol,literswater);}
    fprintf(ferr,"Composition of %s in grams and moles, check vol=%f\n",
                              matnames[i],checkvol);
  fprintf(ferr,"%15s%15s%15s\n","Name","Grams","Moles");
  for(j=0;j<compnums[i];j++)
     compsum[i]+=mass[i]*gramvals[i][j];
  for(j=0;j<compnums[i];j++)
    fprintf(ferr,"%15s%15.3e%15.3e\n",compnames[i][j],
             mass[i]*gramvals[i][j]*100/compsum[i],
             mass[i]*compvals[i][j]*100/compsum[i]);
  molwt=bldmolwt(i);
  degrates[i]/=100;
  if (degrates[i]<0) degrates[i]*= -molwt;//only use for molwt now
  mareas[i]/=literswater;
  mvolumes[i]=100/densities[i]; //used to be molwt/densities[i];
  matvolume[i]=mass[i]/densities[i];
  nmoles[i]=mass[i]/100/literswater;}} //used to be mass[i]/molwt/literswater

int calcoccrrncs(char* sstr)//num occurrences of sstr in this level or above
  //additive counter chains beginning at this level; multiplicative counter
  //for propagating a chain up the structure hierarchy
{int i,j,k,no,//multiplicative counter
    acount=0,//additive counter
     kk;
for(i=0;i<numstructures;i++)
  {j=0;
  while((j<numsubs[i])&&(kk=strcmp(subnames[i][j],sstr))!=0)j++;
  if(kk==0)
       {no=nsuboccrrncs[i][j];
       if((k=nstoccrrncs[i])>0)
         {no*=k;
          foundc=1;}      //found the end of the structure chain for this shape
       else
         {no*=calcoccrrncs(stnames[i]);
         loopcount++;
          if(loopcount>MAXLOOP) errproc("Idiot, you have an occurrence
loop","");}
      acount+=no;}}
return acount;}

//builds the molecular weight (from the atwts table) for each material block
//of the input; if the material contains more than one isotope of U, these
//are averaged together, and the individual isotope entries in the material
//components are collapsed into one atomic weight and one symbol using the
//variable Uxnames={"Ua",...}
float bldmolwt(int ndx)
{int j,k,kk,numUs,hasIso=0;
char *p;
float mwt=0;
j=0;
while ((j<compnums[ndx])&&((p=strchr(compnames[ndx][j],'-'))==NULL))j++;
if(p!=NULL)
  {hasIso=1;
  while ((j<compnums[ndx])&&((p=strchr(compnames[ndx][j],'-'))!=NULL))j++;
```

```
  if(j!=compnums[ndx]) errproc("","all isotopes must come last");}
if(hasIso==1)
 {j=compnums[ndx]-1;
 while((p=strchr(compnames[ndx][j],'-'))!=NULL)
  {if(((p-compnames[ndx][j])!=1)||(compnames[ndx][j][0]!='U'))
      errproc(compnames[ndx][j],"is a strange isotope");
    j--;}
 if(j<compnums[ndx]-1)
  {numUs=compnums[ndx]-j-1;
  for (k=0;k<numUs;k++)
    {kk=compnums[ndx]-k-1;
     mwtUxvals[numUwts]+=
        atwts[findatwtindx(compnames[ndx][kk])]*gramvals[ndx][kk];}
  compnums[ndx]-=numUs-1;
  strcpy(compnames[ndx][compnums[ndx]-1],Uxnames[numUwts]);
  atwts[numelements]=mwtUxvals[numUwts];
  strcpy(atnames[numelements],Uxnames[numUwts]);
  numelements++;
  numUwts++;}}
for(j=0;j<compnums[ndx];j++)//cycle through the elements of this material
  mwt+=atwts[findatwtindx(compnames[ndx][j])]*gramvals[ndx][j];
return mwt;}

void bldatwts()//builds the table of atomic weights from the file atwts.in
{int i=0;
if((fin=fopen("atwts.in","r"))==NULL)
  {printf("couldn't open atomic wts input\n");
  exit(0);}
while(fscanf(fin,"%s %f",atnames[i],&atwts[i])!=EOF)i++;
numelements=i;
fclose(fin);}

int findatwtindx(char elname[7]) //finds the atomic wt for the named element
{int i=0;
while((i<numelements)&&(strcmp(elname,atnames[i])!=0))i++;
if (i==numelements)
  errproc(elname," is not in the table of atomic weights");
return i;}
```

2. Documentation of correct results

Table I-1 presents the volume and area of various shapes calculated by volarea using input files "triga.in" and "test in" (Attachment III), with the results presented in output files "triga.out" and "test.out" (Attachment III). The hand calculations differed slightly from the volarea results for the volume of the spherical segment shell but only by less than 1%. The hand calculations confirmed that the volarea results are correct.

Volarea was documented previously, as well as here, using the data from the TRIGA geochemistry calculation, Ref. 21 (MOL.19991118.0050). This documentation is simply to show that the volarea routine works for its intended purpose, which is to calculate the areas and volumes of different waste package componenets.

Table I-1. Comparison of Volarea and Hand Calculation Results to Confirm Volarea Software Routine

Item Name	Shape with Number of Items in Parentheses	Volume				Area			
		Volarea Result		Hand Calculated		Volarea Result		Calculated	
		Volume All Items	Volume 1 Item	Volume Equation[a]	Volume	Area All Items	Area 1 Item	Area Equation[a]	Area
sstubes	cylinder shell (111)	88401	796	volume=Pi*rout^2*L-Pi*(rout-thickness)^2*L	796	319297	2877	area=2*Pi*rout*L+2*Pi*(rout-thickness)*L	2877
baseplate	cyldinder solid (3)	4062	1354	volume=Pi*r^2*L	1354	8933	2978	area=2*Pi*r*L+2*Pi*r^2	2978
bracket	box solid (36)	3970	110	volume=L1*L2*L3	110	11400	317	area=2*L1*L2+2*L1*L3+2*L2*L3	317
fitting	conefrustrum solid (222)	7453	34	volume=1/3*(areabase+areatop+(areabase*areatop)^(1/2))*alt	34	14619	66	area=PI()*rbase^2+PI()*rtop^2+1/2*(2*PI()*rbase+2*PI()*rtop)*(alt^2+(rbase-rtop)^2)^(1/2)	66
impactplates 2	sphereseg solid (2)	8426	4213	volume=1/6*PI()*alt*(3*rtop^2+3*rbottom^2+alt^2)	4213	6382	3191	R (radius of circle)=sqrt(1/(4*alt^2)*(rbot^2-rtop^2+alt^2)^2+rtop^2) area=2*PI*R*alt+PI*(rbot^2+rtop^2)	45 3191
dishheadsph	sphereseg shell (2) (like a cap)	2995	1498	Rout(radius of outer circle)=sqrt(1/(4*alt^2)*(rbot^2-rtop^2+alt^2)^2+rtop^2) volume=1/3*PI*alt^2*(3*Rout-alt)-1/3*PI*(alt-t)^2*(3*(Rout-t)-(alt-t))-1/2*b*h*2*PI*(r-t)	47 1487	6389	3194	area=2*PI*Rout*alt+2*PI*(Rout-t)*(alt-t)	3194
shape1	cube solid (10)	80	8	volume=side^3	8	240	24	area=6*side^2	24
shape2	cube shell (10)	22	2	volume=side^3-(side-2*t)^3	2	434	43	area=6*side^2+6*(side-2*t)^2	43
shape3	box shell (10)	48	5	volume=L1*L2*L3-(L1-2*t)*(L2-2*t)*(L3-2*t)	5	970	97	area=2*(L1*L2+L1*L3+L2*L3+(L1-2*t)*(L2-2*t)+(L1-2*t)*(L3-2*t)+(L2-2*t)*(L3-2*t))	97
shape4	sphere solid (10)	335	34	volume=4/3*PI()*r3	34	503	50	area=4*PI*r^2	50
shape5	sphere shell (10)	48	5	volume=4/3*PI()*(r^3-(r-t)^3)	5	956	96	area=4*PI*(r^2+(r-t)^2	96
shape6	rtprism solid (10)	400	40	volume=1/2*side^2*length	40	1406	141	area=2*(1/2*side^2)+(side+side+hypotenuse)*length	141

Table I-1. Comparison of Volarea and Hand Calculation Results to Confirm Volarea Software Routine (Continued)

Item Name	Shape with Number of Items in Parentheses	Volume				Area			
		Volarea Result		Hand Calculated		Volarea Result		Calculated	
		Volume All Items	Volume 1 Item	Volume Equation[a]	Volume	Area All Items	Area 1 Item	Area Equation[a]	Area
shape7	rtprism shell (10)	125	12	volume=1/2*length*(side^2-(side-t-t/tan(22.5*PI()/180))^2)	12	2498	250	hypotenuseinside=sqrt(2*(side-t-t/tan(22.5*PI()/180))^2) area=(side+side+hypotenuse)*length+(side-t-t/tan(22.5)+side-t-t/tan(22.5)+hypotenuseinside)*length	2 250
shape8	etprism solid (10)	346	35	volume=1/4*side ^2*(3^(1/2))*length	35	1234	123	area=3*side*length+2*1/4*side^2*(3^(1/2))	123
shape9	etprism shell (10)	110	11	volume=3^(1/2)/4*length*(side^2-(side-2*t*3^(1/2))^2)	11	2192	219	area=3*length*(side+side-2*t*3^(1/2))	219
shape10	hprism solid (10)	2079	208	volume=3/2*side ^2*(3^(1/2))*length	208	2607	261	area=3*side ^2*(3^(1/2))+6*side*length	261
shape11	hprism shell (10)	233	23	volume=3/2*3^(1/2)*length*(side ^2-(side-2*t/3^(1/2))^2)	23	4661	466	area=6*length*(side+side-2*t/(3^(1/2)))	466
shape12	helix solid (10)	124	12	volume=#turns*2*PI^2*larger*smallr^2	12	2472	247	area=#turns*4*pi^2*larger*smallr	247
shape13	conefrustum shell (10)	154	15	a (horizontal thickness)=t/sin(invtan(h/(rbot-rtop))) volume= 1/3*Pi*H*((rbot^2+rtop^2+rbot*rtop)-((rbot-a)^2+(rtop-a)^2+(rtop-a)*(rbot-a))	0.20 15	1537	154	s (slant height) =(alt^2+(rbase-rtop)^2)^(1/2) area=1/2*s*(2*PI()*rbase+2*PI()*rtop+2*PI()*(rbase-a)+2*PI()*(rtop-a))	5 154

Source: [a]References 64 and 16

3. Sample input file: triga.in

```
structure=fuelrods
component=trigaIA 111
occurrences=1

structure=trigaIA
component=fuel 1
component=centerrod 1
component=upperreflector 1
component=lowerreflector 1
component=cladding 1
component=fitting 2


$literswater=4100

shape=fuel
type=cylinder shell
length=38.1
radius=1.82245
thickness=1.50495
matname=UZrHFLIP

shape=centerrod
type=cylinder solid
length=38.1
radius=0.28575
matname=zirc

shape=upperreflector
type=cylinder solid
length=6.5024
radius=1.82245
matname=graphite

shape=lowerreflector
type=cylinder solid
length=9.4488
radius=1.82245
matname=graphite

shape=cladding
type=cylinder shell
length=57.531
radius=1.87706
thickness=0.0508
matname=304LSSC

shape=fitting
type=conefrustrum solid
bottomrad=1.87706
toprad=0.01
altitude=9.05
```

```
matname=304LSSD

*     DOE Canister

shape=outer18pipe
type=cylinder shell
length=299.9
radius=22.86
thickness=0.9525
matname=316LSSE
occurrences=1

shape=dishheadsph
type=sphereseg shell
altitude=5.94
largerad=22.86
smallrad=0.001
thickness=0.9525
matname=316LSSE
occurrences=2

shape=plugplates
type=cylinder solid
length=0.64
radius=3.34
matname=316LSSE
occurrences=2

shape=plugs
type=cylinder solid
length=1.27
radius=1.27
matname=316LSSE
occurrences=2

shape=liftingrings
type=cylinder shell
length=1.27
radius=21.755
thickness=2.5399
matname=316LSSE
occurrences=2

shape=backingring
type=cylinder shell
length=5.08
radius=21.905
thickness=0.47752
matname=316LSSE
occurrences=1

structure=impactplate
component=impactplates1 1
component=impactplates2 1
component=impactplatemeet -1
occurrences=2
```

```
shape=impactplates1
type=cylinder solid
length=0.9144
radius=21.275
matname=A516Grade70

shape=impactplates2
type=sphereseg solid
altitude=4.17
largerad=22.19
smallrad=12.04
matname=A516Grade70

shape=impactplatemeet
type=cylinder solid
length=0.001
radius=21.275
matname=A516Grade70


*     Basket Structure

shape=sstubes
type=cylinder shell
length=83.6
radius=3.015
thickness=0.55372
matname=316LSSG
occurrences=111


shape=baseplate
type=cylinder solid
length=0.95
radius=21.3
matname=316LSSG
occurrences=3

shape=abstubes
type=cylinder shell
length=83.6
radius=2.46
thickness=0.1
matname=alloy22Gd
occurrences=45

shape=bracket
type=box solid
side1=10.798
side2=0.79
side3=12.928
matname=316LSSG
occurrences=36

*     Material Descriptions

material=alloy22Gd
```

```
density=8.534171
degrate=2.7043E-12 grams
numelements=10
C=0.012415727
P=0.016554303
S=0.016554303
Si=0.066217212
Cr=17.58894707
Mn=0.413857578
Fe=5.589382029
Ni=45.32982052
Mo=12.4699554
Gd=18.49629586

material=UZrHFLIP
density=5.947
degrate=1.8928E-12 grams
numelements=4
H=1.588616303
Zr=89.86145852
U-238=2.5737
U-235=5.9762

material=zirc
density=6.49
degrate=4.0E-14 grams
numelements=1
Zr=100

material=graphite
density=2.25
degrate=4.0E-14 grams
numelements=1
C=100

material=A516Grade70
density=7.850
degrate=8.7063E-10 grams
numelements=6
C=0.28
Mn=1.045
P=0.035
S=0.035
Si=0.29
Fe=98.315

material=316LSSE
density=7.980
degrate=2.52871E-12 grams
numelements=10
C=0.03
Mn=2.0
P=0.045
S=0.03
Si=1.0
Cr=17.0
Ni=12.0
```

```
Mo=2.5
N=0.1
Fe=65.295

material=316LSSG
density=7.980
degrate=2.52871E-12 grams
numelements=10
C=0.03
Mn=2.0
P=0.045
S=0.03
Si=1.0
Cr=17.0
Ni=12.0
Mo=2.5
N=0.1
Fe=65.295

material=304LSSC
density=7.940
degrate=2.51603E-12 grams
numelements=9
C=0.03
Mn=2.0
P=0.045
S=0.03
Si=0.75
Cr=19.0
Ni=10.0
N=0.1
Fe=68.045

material=304LSSD
density=7.940
degrate=2.51603E-12 grams
numelements=9
C=0.03
Mn=2.0
P=0.045
S=0.03
Si=0.75
Cr=19.0
Ni=10.0
N=0.1
Fe=68.045
```

Sample input file: test.in

```
structure=assembly
component=shape1 10
component=shape2 10
component=shape3 10
component=shape4 10
component=shape5 10
component=shape6 10
component=shape7 10
component=shape8 10
component=shape9 10
component=shape10 10
component=shape11 10
component=shape12 10
component=shape13 10
occurrences=1

shape=shape1
type=cube solid
side=2.0
matname=316LSS

shape=shape2
type=cube shell
side=2.0
thickness=0.1
matname=316LSS

shape=shape3
type=box shell
side1=2.0
side2=3.0
side3=4.0
thickness=0.1
matname=316LSS

shape=shape4
type=sphere solid
radius=2.0
matname=316LSS

shape=shape5
type=sphere shell
radius=2.0
thickness=0.1
matname=316LSS

shape=shape6
type=rtprism solid
side=2.0
length=20.0
matname=316LSS
```

```
shape=shape7
type=rtprism shell
side=2.0
length=20.0
thickness=0.1
matname=316LSS

shape=shape8
type=etprism solid
side=2.0
length=20.0
matname=316LSS

shape=shape9
type=etprism shell
side=2.0
length=20.0
thickness=0.1
matname=316LSS

shape=shape10
type=hprism solid
side=2.0
length=20.0
matname=316LSS

shape=shape11
type=hprism shell
side=2.0
length=20.0
thickness=0.1
matname=316LSS

shape=shape12
type=helix solid
altitude=25.0
smallradius=0.1
largeradius=0.5
turns=125
matname=316LSS

shape=shape13
type=conefrustrum shell
altitude=5.0
bottomrad=3.0
toprad=2.0
thickness=0.2
matname=316LSS

material=316LSS
density=7.980
degrate=2.516E-12 grams
numelements=10
C=0.03
Mn=2.0
P=0.045
S=0.03
```

```
Si=1.0
Cr=17.0
Ni=12.0
Mo=2.5
N=0.1
Fe=65.295
```

4. Sample output file: triga.out

```
*      DOE Canister
*      Basket Structure
*      Material Descriptions

Composition of alloy22Gd in grams and moles, check vol=5696.601074
            Name           Grams           Moles
               C     1.242e-002     1.034e-003
               P     1.655e-002     5.345e-004
               S     1.655e-002     5.163e-004
              Si     6.622e-002     2.358e-003
              Cr     1.759e+001     3.383e-001
              Mn     4.139e-001     7.533e-003
              Fe     5.589e+000     1.001e-001
              Ni     4.533e+001     7.724e-001
              Mo     1.247e+001     1.300e-001
              Gd     1.850e+001     1.176e-001
Composition of UZrHFLIP in grams and moles, check vol=42788.152344
            Name           Grams           Moles
               H     1.589e+000     1.576e+000
              Zr     8.986e+001     9.851e-001
            U-238     2.574e+000     1.081e-002
            U-235     5.976e+000     2.543e-002
Composition of zirc in grams and moles, check vol=1084.851440
            Name           Grams           Moles
              Zr     1.000e+002     1.096e+000
Composition of graphite in grams and moles, check vol=18474.703125
            Name           Grams           Moles
               C     1.000e+002     8.326e+000
Composition of A516Grade70 in grams and moles, check vol=11023.248047
            Name           Grams           Moles
               C     2.800e-001     2.331e-002
              Mn     1.045e+000     1.902e-002
               P     3.500e-002     1.130e-003
               S     3.500e-002     1.091e-003
              Si     2.900e-001     1.033e-002
              Fe     9.832e+001     1.760e+000
Composition of 316LSSE in grams and moles, check vol=44388.121094
            Name           Grams           Moles
               C     3.000e-002     2.498e-003
              Mn     2.000e+000     3.640e-002
               P     4.500e-002     1.453e-003
               S     3.000e-002     9.356e-004
              Si     1.000e+000     3.561e-002
              Cr     1.700e+001     3.269e-001
              Ni     1.200e+001     2.045e-001
              Mo     2.500e+000     2.606e-002
               N     1.000e-001     7.139e-003
              Fe     6.529e+001     1.169e+000
Composition of 316LSSG in grams and moles, check vol=96432.812500
            Name           Grams           Moles
               C     3.000e-002     2.498e-003
              Mn     2.000e+000     3.640e-002
               P     4.500e-002     1.453e-003
               S     3.000e-002     9.356e-004
```

Si	1.000e+000	3.561e-002
Cr	1.700e+001	3.269e-001
Ni	1.200e+001	2.045e-001
Mo	2.500e+000	2.606e-002
N	1.000e-001	7.139e-003
Fe	6.529e+001	1.169e+000

Composition of 304LSSC in grams and moles, check vol=3774.243164

Name	Grams	Moles
C	3.000e-002	2.498e-003
Mn	2.000e+000	3.640e-002
P	4.500e-002	1.453e-003
S	3.000e-002	9.356e-004
Si	7.500e-001	2.670e-002
Cr	1.900e+001	3.654e-001
Ni	1.000e+001	1.704e-001
N	1.000e-001	7.139e-003
Fe	6.804e+001	1.218e+000

Composition of 304LSSD in grams and moles, check vol=7452.574707

Name	Grams	Moles
C	3.000e-002	2.498e-003
Mn	2.000e+000	3.640e-002
P	4.500e-002	1.453e-003
S	3.000e-002	9.356e-004
Si	7.500e-001	2.670e-002
Cr	1.900e+001	3.654e-001
Ni	1.000e+001	1.704e-001
N	1.000e-001	7.139e-003
Fe	6.805e+001	1.218e+000

BY SHAPE
fuel Area=56863.218750 Volume=42788.152344 Material=UZrHFLIP
centerrod Area=7649.958984 Volume=1084.851440 Material=zirc
upperreflector Area=10581.199219 Volume=7531.088867 Material=graphite
lowerreflector Area=14326.184570 Volume=10943.614258 Material=graphite
cladding Area=148592.203125 Volume=3774.243164 Material=304LSSC
fitting Area=14618.901367 Volume=7452.574707 Material=304LSSD
outer18pipe Area=84356.625000 Volume=40174.828125 Material=316LSSE
dishheadsph Area=6388.553711 Volume=2994.970459 Material=316LSSE
plugplates Area=167.047272 Volume=44.859325 Material=316LSSE
plugs Area=40.536598 Volume=12.870369 Material=316LSSE
liftingrings Area=653.853699 Volume=830.361572 Material=316LSSE
backingring Area=1383.111328 Volume=330.231842 Material=316LSSE
impactplates1 Area=5932.325684 Volume=2600.489990 Material=A516Grade70
impactplates2 Area=6382.131348 Volume=8425.601563 Material=A516Grade70
impactplatemeet Area=-5688.128418 Volume=-2.843931 Material=A516Grade70
sstubes Area=319296.937500 Volume=88400.554688 Material=316LSSG
baseplate Area=8933.275391 Volume=4062.130859 Material=316LSSG
abstubes Area=113931.992188 Volume=5696.601074 Material=alloy22Gd
bracket Area=11400.486328 Volume=3970.125977 Material=316LSSG

BY MATERIAL
alloy22Gd Density=8.53417 Moles=0.118575 Area=27.7883 Volume=5696.6
UZrHFLIP Density=5.947 Moles=0.620637 Area=13.8691 Volume=42788.2
zirc Density=6.49 Moles=0.0171724 Area=1.86584 Volume=1084.85
graphite Density=2.25 Moles=0.101386 Area=6.07497 Volume=18474.7
A516Grade70 Density=7.85 Moles=0.211055 Area=1.61618 Volume=11023.2
316LSSE Density=7.98 Moles=0.863944 Area=22.6804 Volume=44388.1

```
316LSSG Density=7.98 Moles=1.87691 Area=82.8368 Volume=96432.8
304LSSC Density=7.94 Moles=0.0730914 Area=36.242 Volume=3774.24
304LSSD Density=7.94 Moles=0.144325 Area=3.56559 Volume=7452.57
```

Sample output file: test.out

```
Composition of 316LSS in grams and moles, check vol=4102.795410
           Name          Grams          Moles
              C     3.000e-002     2.498e-003
             Mn     2.000e+000     3.640e-002
              P     4.500e-002     1.453e-003
              S     3.000e-002     9.356e-004
             Si     1.000e+000     3.561e-002
             Cr     1.700e+001     3.269e-001
             Ni     1.200e+001     2.045e-001
             Mo     2.500e+000     2.606e-002
              N     1.000e-001     7.139e-003
             Fe     6.529e+001     1.169e+000

BY SHAPE
shape1 Area=240.000000 Volume=80.000000 Material=316LSS
shape2 Area=434.399994 Volume=21.680000 Material=316LSS
shape3 Area=970.400024 Volume=48.480000 Material=316LSS
shape4 Area=502.654846 Volume=335.103210 Material=316LSS
shape5 Area=956.300781 Volume=47.794109 Material=316LSS
shape6 Area=1405.685425 Volume=400.000000 Material=316LSS
shape7 Area=2498.233887 Volume=124.911690 Material=316LSS
shape8 Area=1234.640991 Volume=346.410187 Material=316LSS
shape9 Area=2192.153809 Volume=109.607712 Material=316LSS
shape10 Area=2607.846191 Volume=2078.460938 Material=316LSS
shape11 Area=4661.436035 Volume=233.071808 Material=316LSS
shape12 Area=2472.395996 Volume=123.619804 Material=316LSS
shape13 Area=1536.559082 Volume=153.655930 Material=316LSS

BY MATERIAL
316LSS Density=7.98 Moles=0.0831605 Area=5.51504 Volume=4102.8
```

File: atwts.in

```
H        1.00794
He        4.0026
Li         6.941
B         10.811
C        12.0107
N       14.00674
O        15.9994
F        18.9984
Na      22.98977
Mg         24.305
Al      26.98154
Si       28.0855
P       30.97376
S          32.066
Cl       35.4527
K        39.0983
Ca         40.078
Ti         47.867
V        50.9415
Cr       51.9961
Mn      54.93805
Fe         55.845
Co       58.9332
Ni           58.69
Cu         63.546
Zn           65.39
As      74.92160
Sr           87.62
Zr         91.224
Nb      92.90638
Mo           95.94
Tc      98.90628
Ru          101.07
Rh      102.9055
Ag      107.8682
Cd       112.411
In       114.818
Sn         118.71
Cs      132.9054
Ba       137.327
La      138.9055
Ce       140.116
Nd         144.24
Sm         150.36
Eu       151.964
Gd         157.25
Hf         178.49
Ta      180.9479
W          183.84
Pb           207.2
Th      232.0381
```

U	238.0289
U-233	233.0396
U-234	234.0409
U-235	235.0439
U-236	236.0456
U-238	238.0508
Np	237.048
Pu	239.0521
Er	167.26

ATTACHMENT II. LISTING OF FILES ON COMPACT DISKS

This attachment contains the MS-DOS directory for files placed on the electronic media (Attachment III, two compact disks). The files are of various types:

1) Excel files (extension = xls).
2) EQ3/6 input files (extensions = 3i or 6i).
3) EQ6 output files (text, extension = 6o).
4) Tab-delimited text files (extension = txt), with names n???????.elem????.txt. These contain total aqueous moles (*.elem_aqu.txt), total moles in minerals and aqueous phase (*.elem_m_a.txt), total moles in minerals, aqueous phase, and remain special reactants (*.elem_tot.txt), and the total moles in minerals alone (*.elem_min.txt). The *.elem_tot.txt and *.elem_min.txt also have the volume in cm^3 of the minerals and total solids (including special reactants) in the system.
5) EQ6 text data file used for the calculations, named data0.ymp.
6) Selected binary files (bin extension), created by EQ6, used for plotting.
7) Figures created by the plotting program (pp.exe, Ref. 30)with files names such as *.wmf and wmf.*.

Below are listed the contents of the DOS directories within the electronic attachment:

The first column is the DOS file name.
The second column lists <DIR> if it is a folder or gives the file size (bytes) if it is a file.
The third and fourth columns are the date and time of the last update.
The fifth column is the file name.

```
Directory of N-Reactor 2

A516_R~6 XLS        26,624  12-11-00  1:41p A516_Rate.xls
DATA0    NUC     2,305,224  10-04-99  7:38a data0.nuc
DATA0    YMP     2,675,993  09-13-00  4:54p data0.ymp
N-REA~26 DOC        31,232  09-06-00  2:28p N-reactor_15thEd.doc
N-REA~30 DOC    11,965,440  09-11-00  3:29p N-Reactor_Tables&Plots.doc
N10#1111 6I         48,815  07-27-00  8:19a N10#1111.6i
N10#1111 6O      1,804,056  07-27-00  8:27a n10#1111.6o
N10#1111 6P         48,322  07-27-00  8:27a n10#1111.6p
N10#1111 BIN    11,257,304  07-27-00  8:27a N10#1111.bin
N10#~114 TXT        17,500  07-27-00  8:27a N10#1111.elem_aqu.txt
N10#~116 TXT        16,355  07-27-00  8:27a N10#1111.elem_min.txt
N10#~118 TXT        16,368  07-27-00  8:27a N10#1111.elem_tot.txt
N10#1111 TXT        41,784  07-27-00  1:40p N10#1111.TXT
N10#~122 TXT        34,407  07-27-00  8:43a N10#1111_min_info.txt
N10#~124 WMF       140,140  07-27-00 11:07a N10#1111a.wmf
N10#~126 WMF       264,536  07-27-00  1:34p N10#1111b.wmf
N10&1111 6I         48,889  07-27-00  4:46p N10&1111.6i
N10&1111 6O        420,946  07-27-00  4:47p n10&1111.6o
N10&1111 6P         48,224  07-27-00  4:47p n10&1111.6p
N10&1111 BIN       187,880  07-27-00  4:47p N10&1111.bin
N10&~138 TXT         4,504  07-27-00  4:47p N10&1111.elem_aqu.txt
N10&~140 TXT         4,223  07-27-00  4:47p N10&1111.elem_min.txt
N10&~142 TXT         4,236  07-27-00  4:47p N10&1111.elem_tot.txt
N10&1111 TXT           663  07-27-00  5:21p N10&1111.TXT
N10&1111 WMF       270,232  07-27-00  5:19p N10&1111.wmf
N10A1111 6I         42,436  07-11-00  3:25p N10A1111.6i
N10A1111 6O        308,743  07-11-00  3:26p n10a1111.6o
N10A1111 6P         41,587  07-11-00  3:26p n10a1111.6p
N10A1111 BIN       301,376  07-11-00  3:26p N10A1111.bin
```

```
N10A~160 TXT          3,316  07-11-00  3:26p N10A1111.elem_aqu.txt
N10A~162 TXT          3,107  07-11-00  3:26p N10A1111.elem_min.txt
N10A~164 TXT          3,120  07-11-00  3:26p N10A1111.elem_tot.txt
N10A1201 6I          42,510  08-09-00  2:49p N10A1201.6i
N10A1201 6O       1,696,437  08-09-00  2:53p n10a1201.6o
N10A1201 6P          42,235  08-09-00  2:53p n10a1201.6p
N10A1201 BIN      1,962,072  08-09-00  2:53p N10A1201.bin
N10A~184 TXT         17,974  08-09-00  2:53p N10A1201.elem_aqu.txt
N10A~186 TXT         16,757  08-09-00  2:53p N10A1201.elem_min.txt
N10A~188 TXT         16,770  08-09-00  2:53p N10A1201.elem_tot.txt
N10A~190 XLS         56,832  07-25-00  8:21a N10A1201.elem_tot.xls
N10A1201 TX0         18,279  07-19-00  2:17p N10A1201.TX0
N10A1201 TXT         21,839  07-18-00  4:50p N10A1201.TXT
N10A~198 TXT         44,365  08-09-00  1:54p N10A1201_min_info.txt
N10A~200 WMF        132,062  07-19-00  1:16p N10A1201a.wmf
N10A~202 WMF        130,472  07-19-00  1:27p N10A1201b.wmf
N10A~204 WMF        139,284  07-24-00  6:31p N10A1201c.wmf
N10B1011 6I          45,125  08-09-00  3:10p n10b1011.6i
N10B1011 6O       1,294,074  08-09-00  3:15p n10b1011.6o
N10B1011 6P          44,724  08-09-00  3:15p n10b1011.6p
N10B1011 BIN      9,715,888  08-09-00  3:14p N10B1011.bin
N10B~246 TXT         12,085  08-09-00  3:14p N10B1011.elem_aqu.txt
N10B~248 TXT         11,300  08-09-00  3:14p N10B1011.elem_min.txt
N10B~250 TXT         11,313  08-09-00  3:14p N10B1011.elem_tot.txt
N10B1011 TXT         89,088  07-20-00  6:50p N10B1011.TXT
N10B1011 TXU        124,229  07-20-00  6:51p N10B1011.TXU
N10B~256 WMF        204,640  07-20-00  6:08p N10B1011a.wmf
N10B~258 WMF        134,240  07-20-00  6:22p N10B1011b.wmf
N10G2111 6I          49,333  08-10-00 11:09a N10g2111.6i
N10G2111 6O       2,407,190  08-10-00 11:18a n10g2111.6o
N10G2111 6P          49,390  08-10-00 11:18a n10g2111.6p
N10G2111 BIN     11,837,768  08-10-00 11:18a N10G2111.bin
N10G~312 TXT         23,637  08-10-00 11:18a N10G2111.elem_aqu.txt
N10G~314 TXT         22,084  08-10-00 11:18a N10G2111.elem_min.txt
N10G~316 TXT         22,097  08-10-00 11:18a N10G2111.elem_tot.txt
N10G~318 TXT         38,279  08-10-00 11:05a N10g2111_min_info.txt
N10H1111 6I          48,741  07-19-00  5:19p N10h1111.6i
N10H1111 6O       1,864,458  07-19-00  5:32p n10h1111.6o
N10H1111 6P          48,174  07-19-00  5:32p n10h1111.6p
N10H1111 BIN     11,343,536  07-19-00  5:31p N10H1111.bin
N10H~366 TXT         18,222  07-19-00  5:31p N10H1111.elem_aqu.txt
N10H~368 TXT         17,029  07-19-00  5:31p N10H1111.elem_min.txt
N10H~370 TXT         17,042  07-19-00  5:31p N10H1111.elem_tot.txt
N10H1111 TXT        163,780  07-24-00  1:23p N10H1111.TXT
N10H~374 TXT         35,399  07-19-00  5:33p N10h1111_min_info.txt
N10H~378 WMF        260,586  07-19-00  6:19p N10h1111a.wmf
N10H~380 WMF        126,900  07-19-00  6:34p N10h1111b.wmf
N10H1112 6I          48,963  07-26-00  8:15a N10h1112.6i
N10H1112 6O       7,473,929  07-26-00  3:39p n10h1112.6o
N10H1112 6P          48,372  07-26-00  3:39p n10h1112.6p
N10H1112 BIN              0  07-26-00  3:39p N10H1112.bin
N10H~412 TXT         63,347  07-26-00  3:39p N10H1112.elem_aqu.txt
N10H~414 TXT         59,154  07-26-00  2:39p N10H1112.elem_min.txt
N10H~416 TXT         59,167  07-26-00  2:39p N10H1112.elem_tot.txt
N10H1112 TXT        303,549  07-26-00  4:33p N10H1112.TXT
N10H~422 TXT        116,595  07-26-00  2:43p N10h1112_min_info.txt
N10H~424 WMF        149,164  07-26-00  5:04p N10h1112a.wmf
```

```
N10H~426 WMF       136,302  07-26-00  5:16p N10h1112b.wmf
N10H1211 6I         49,141  08-03-00  9:31a N10h1211.6i
N10H1211 6O      2,566,252  08-03-00  2:39p n10h1211.6o
N10H1211 6P         49,196  08-03-00  2:39p n10h1211.6p
N10H1211 BIN    12,468,736  08-03-00  2:39p N10h1211.bin
N10H~482 TXT        24,806  08-03-00  2:39p N10h1211.elem_aqu.txt
N10H~484 TXT        23,277  08-03-00  2:39p N10h1211.elem_min.txt
N10H~486 TXT        23,290  08-03-00  2:39p N10h1211.elem_tot.txt
N10H1211 TXT        43,319  08-03-00  3:54p N10H1211.TXT
N10H~490 TXT        41,156  08-03-00  2:41p N10h1211_min_info.txt
N10H2111 6I         48,815  07-24-00  2:15p N10h2111.6i
N10H2111 6O      2,691,047  07-24-00  3:27p n10h2111.6o
N10H2111 6P         48,528  08-09-00 12:25p n10h2111.6p
N10H2111 BIN     4,403,776  08-09-00 12:25p N10h2111.bin
N10H~520 TXT        18,944  08-09-00 12:25p N10h2111.elem_aqu.txt
N10H~522 TXT        17,703  08-09-00 12:25p N10h2111.elem_min.txt
N10H~524 TXT        17,716  08-09-00 12:25p N10h2111.elem_tot.txt
N10H2111 TXT       384,883  07-24-00  5:11p N10H2111.TXT
N10H~530 TXT        59,043  07-24-00  3:06p N10h2111_min_info.txt
N10H~532 WMF       183,422  07-25-00 10:27a N10h2111a.wmf
N10H~534 WMF       222,866  07-25-00  9:42a N10h2111b.wmf
N10H~538 WMF       113,550  07-25-00 10:12a N10h2111c.wmf
N11&1111 6I         47,007  07-27-00  4:56p n11&1111.6i
N11&1111 6O      1,446,456  07-27-00  5:01p n11&1111.6o
N11&1111 6P         47,409  07-27-00  5:01p n11&1111.6p
N11&1111 BIN    10,179,920  07-27-00  5:01p N11&1111.bin
N11&~582 TXT        13,890  07-27-00  5:01p N11&1111.elem_aqu.txt
N11&~584 TXT        12,985  07-27-00  5:01p N11&1111.elem_min.txt
N11&~586 TXT        12,998  07-27-00  5:01p N11&1111.elem_tot.txt
N11&1111 TXT        38,139  07-27-00  5:21p N11&1111.TXT
N11A1111 6I         40,444  07-11-00  4:25p n11a1111.6i
N11A1111 6O      1,443,415  07-17-00 10:01a n11a1111.6o
N11A1111 6P         41,166  07-17-00 10:01a n11a1111.6p
N11A1111 BIN     9,400,856  07-17-00 10:01a N11A1111.bin
N11A~630 TXT        14,484  07-17-00 10:01a N11A1111.elem_aqu.txt
N11A~632 TXT        13,507  07-17-00 10:01a N11A1111.elem_min.txt
N11A~634 TXT        13,520  07-17-00 10:01a N11A1111.elem_tot.txt
N11A1211 6I         41,593  07-11-00  2:52p n11a1211.6i
N11H1112 6I         39,713  07-26-00  2:07p n11h1112.6i
N11H1112 6O        161,000  07-26-00  2:44p n11h1112.6o
N11H1112 6P         40,017  07-26-00  2:44p n11h1112.6p
N11H1112 BIN       234,752  07-26-00  2:44p N11H1112.bin
N11H~648 TXT          1,616  07-26-00  2:44p N11H1112.elem_aqu.txt
N11H~650 TXT          1,527  07-26-00  2:44p N11H1112.elem_min.txt
N11H~652 TXT          1,540  07-26-00  2:44p N11H1112.elem_tot.txt
N11H~654 TXT          4,272  07-26-00  2:45p N11h1112_min_info.txt
N11H2111 6I         38,270  08-09-00 12:37p n11h2111.6i
N11H2111 6O        997,595  08-09-00 11:43a n11h2111.6o
N11H2111 6P         38,348  08-09-00 11:43a n11h2111.6p
N11H2111 BIN     7,289,904  08-09-00 11:43a N11h2111.bin
N11H~688 TXT          8,603  08-09-00 11:43a N11h2111.elem_aqu.txt
N11H~690 TXT          8,010  08-09-00 11:43a N11h2111.elem_min.txt
N11H~692 TXT          8,023  08-09-00 11:43a N11h2111.elem_tot.txt
N11H~694 TXT         11,282  08-08-00 12:17p N11h2111_min_info.txt
N12H1112 6I         40,091  07-26-00  2:09p n12h1112.6i
N12H1112 6O        396,602  07-26-00  2:11p n12h1112.6o
N12H1112 6P         40,165  07-26-00  2:11p n12h1112.6p
```

```
N12H1112 BIN      2,483,104  07-26-00   2:11p N12H1112.bin
N12H~714 TXT          3,782  07-26-00   2:11p N12H1112.elem_aqu.txt
N12H~716 TXT          3,549  07-26-00   2:11p N12H1112.elem_min.txt
N12H~718 TXT          3,562  07-26-00   2:11p N12H1112.elem_tot.txt
N12H1112 TXT          9,357  07-26-00   4:34p N12H1112.TXT
N12H1112 WMF        160,764  07-26-00   5:24p N12h1112.wmf
N12H~724 TXT          7,660  07-26-00   2:15p N12h1112_min_info.txt
N12H2111 6I          39,404  08-08-00  10:37a n12h2111.6i
N12H2111 6O         462,165  08-08-00  10:38a n12h2111.6o
N12H2111 6P          39,552  08-08-00  10:38a n12h2111.6p
N12H2111 BIN      1,445,192  08-08-00  10:38a N12h2111.bin
N12H~740 TXT          5,226  08-08-00  10:38a N12h2111.elem_aqu.txt
N12H~742 TXT          4,897  08-08-00  10:38a N12h2111.elem_min.txt
N12H~744 TXT          4,910  08-08-00  10:38a N12h2111.elem_tot.txt
N13H2111 6I          39,626  08-08-00  10:42a n13h2111.6i
N13H2111 6O       1,055,260  08-08-00  10:47a n13h2111.6o
N13H2111 6P          39,700  08-08-00  10:47a n13h2111.6p
N13H2111 BIN      7,010,160  08-08-00  11:47a N13h2111.bin
N13H~778 TXT         11,363  08-08-00  11:47a N13h2111.elem_aqu.txt
N13H~780 TXT         10,626  08-08-00  10:47a N13h2111.elem_min.txt
N13H~782 TXT         10,639  08-08-00  10:47a N13h2111.elem_tot.txt
N40H1111 6I          47,617  07-31-00  12:20p N40h1111.6i
N40H1111 6O       2,652,944  07-31-00  12:55p n40h1111.6o
N40H1111 6P          46,977  07-31-00  12:55p n40h1111.6p
N40H1111 BIN     22,624,680  07-31-00  12:55p N40h1111.bin
N40H~866 TXT         24,720  07-31-00  12:55p N40h1111.elem_aqu.txt
N40H~868 TXT         23,095  07-31-00  12:55p N40h1111.elem_min.txt
N40H~870 TXT         23,108  07-31-00  12:55p N40h1111.elem_tot.txt
N40H1111 TXT         84,174  07-31-00   1:30p N40H1111.TXT
N40H~874 TXT         45,575  07-31-00   1:19p N40h1111_min_info.txt
N40H1112 6I          47,913  07-31-00   5:53p N40h1112.6i
N40H1112 6O       7,494,087  08-01-00   9:32a n40h1112.6o
N40H1112 6P          47,323  08-01-00   9:32a n40h1112.6p
N40H1112 BIN     81,716,160  08-01-00  10:32a N40h1112.bin
N40~1146 TXT         64,069  08-01-00   9:32a N40h1112.elem_aqu.txt
N40~1148 TXT         59,828  08-01-00   9:32a N40h1112.elem_min.txt
N40~1150 TXT         59,841  08-01-00   9:32a N40h1112.elem_tot.txt
N40H1112 TXT         30,440  08-01-00   9:59a N40H1112.TXT
N40~1154 TXT        121,789  08-01-00   9:34a N40h1112_min_info.txt
N40H2111 6I          47,691  07-31-00  12:21p N40h2111.6i
N40H2111 6O       3,359,190  08-03-00   8:45a n40h2111.6o
N40H2111 6P          47,371  08-03-00   8:45a n40h2111.6p
N40H2111 BIN     23,903,840  08-03-00   8:45a N40h2111.bin
N40~1244 TXT         31,940  08-03-00   8:45a N40h2111.elem_aqu.txt
N40~1246 TXT         29,835  08-03-00   8:45a N40h2111.elem_min.txt
N40~1248 TXT         29,848  08-03-00   8:45a N40h2111.elem_tot.txt
N40H2111 TXT         88,521  07-31-00   1:49p N40H2111.TXT
N40~1252 TXT         66,595  07-31-00  12:46p N40h2111_min_info.txt
N41H1112 6I          39,565  08-01-00   8:56a n41h1112.6i
N41H1112 6O         160,702  08-01-00   8:57a n41h1112.6o
N41H1112 6P          39,869  08-01-00   8:57a n41h1112.6p
N41H1112 BIN        234,752  08-01-00   8:57a N41h1112.bin
N41~1264 TXT          1,616  08-01-00   8:57a N41h1112.elem_aqu.txt
N41~1266 TXT          1,527  08-01-00   8:57a N41h1112.elem_min.txt
N41~1268 TXT          1,540  08-01-00   8:57a N41h1112.elem_tot.txt
N41~1270 TXT          4,272  08-01-00   8:58a N41h1112_min_info.txt
N42H1112 6I          39,943  08-01-00   9:02a n42h1112.6i
```

```
N42H1112 6O          448,559  08-01-00  9:03a n42h1112.6o
N42H1112 6P           40,017  08-01-00  9:03a n42h1112.6p
N42H1112 BIN       2,483,104  08-01-00  9:03a N42h1112.bin
N42~1288 TXT           4,504  08-01-00  9:03a N42h1112.elem_aqu.txt
N42~1290 TXT           4,223  08-01-00  9:03a N42h1112.elem_min.txt
N42~1292 TXT           4,236  08-01-00  9:03a N42h1112.elem_tot.txt
N42H1112 TXT           9,353  08-01-00 10:05a N42H1112.TXT
N42~1296 TXT           8,724  08-01-00  9:04a n42h1112_min_info.txt
NREACTOR XLS         143,872  01-16-01 11:04a NReactor.xls
NRE~1304 XLS       4,894,208  12-18-00  4:50p NReactor_U.xls
VOLAREA         <DIR>         01-16-01 11:21a volarea
WMF      022           345,912  07-28-00  1:48p WMF.022
WMF      023           346,812  07-28-00  1:49p WMF.023
WMF      024           108,966  07-28-00  1:56p WMF.024
WMF      025           343,092  07-28-00  2:03p WMF.025
WMF      029           383,626  07-31-00  1:41p WMF.029
WMF      030           141,032  07-31-00  1:46p WMF.030
WMF      031           328,016  07-31-00  1:58p WMF.031
WMF      032           241,960  07-31-00  2:10p WMF.032
WMF      033           118,088  07-31-00  2:15p WMF.033
WMF      034           224,124  08-01-00  9:53a WMF.034
WMF      035           117,930  08-01-00  9:58a WMF.035
WMF      036           158,884  08-01-00 10:05a WMF.036
WMF      037           332,270  08-03-00  3:43p WMF.037
WMF      038           161,906  08-03-00  3:53p WMF.038
       224 file(s)    308,519,821 bytes

Directory of D:\volarea

.               <DIR>         08-03-00  3:53p .
..              <DIR>         08-03-00  3:53p ..
ATWTS    IN           1,020  11-29-00  1:19p atwts.in
DATAMIA  IN           3,045  07-06-00 10:22a dataMIA.in
DATAMIA  OUT          4,337  07-06-00 10:24a dataMIA.out
DATAMIV  IN           2,885  07-06-00 10:43a dataMIV.in
DATAMIV  OUT          3,918  07-06-00 10:44a dataMIV.out
RUNVOL   BAT             11  11-29-00 11:29a runvol.bat
TEST     IN           1,565  11-29-00 11:27a test.in
TEST     OUT          1,434  11-29-00  1:39p test.out
TEST     TXT          1,565  11-29-00 11:27a test.txt
TRIGA    IN           3,978  11-29-00 11:30a triga.in
TRIGA    OUT          5,990  11-29-00 11:30a Triga.out
TRIGA    TXT          3,978  11-29-00 11:27a Triga.txt
VOLAR~30 XLS         30,208  11-29-00  2:16p volarea qualify.xls
VOLAREA  C           34,054  05-18-00 11:05a volarea.c
VOLAREA  EXE        229,428  05-18-00 11:04a volarea.exe
        15 file(s)        327,416 bytes

Total files listed:
       239 file(s)    308,847,237 bytes
```